

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM083024\
 Data File : BM047411.D
 Acq On : 30 Aug 2024 18:19
 Operator : RC/JU
 Sample : P3795-03
 Misc :
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 239

Integration Parameters: rteint.p

Integrator: RTE

Smoothing : ON

Filtering: 5

Sampling : 1

Min Area: 3 % of largest Peak

Start Thrs: 0.2

Max Peaks: 100

Stop Thrs : 0

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM082624.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM047411.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.557	276	284	292	rBV	129282	194751	1.71%	0.108%
2	5.004	354	360	378	rBV	2154563	3233339	28.46%	1.793%
3	6.569	620	626	650	rVB	1906236	3266355	28.76%	1.812%
4	7.340	748	757	768	rBV	759099	1219435	10.74%	0.676%
5	8.492	946	953	971	rBV	1278152	2197129	19.34%	1.219%
6	9.634	1141	1147	1157	rBV	190194	358900	3.16%	0.199%
7	10.098	1218	1226	1242	rBV	888240	1563063	13.76%	0.867%
8	11.175	1405	1409	1417	rVB2	94130	155900	1.37%	0.086%
9	11.557	1468	1474	1482	rVB	155684	251323	2.21%	0.139%
10	11.680	1490	1495	1499	rVB	124309	194887	1.72%	0.108%
11	11.828	1517	1520	1526	rVB3	119676	175950	1.55%	0.098%
12	12.398	1612	1617	1622	rBV6	82324	144667	1.27%	0.080%
13	12.610	1647	1653	1665	rVB	3499067	5256792	46.28%	2.916%
14	12.745	1671	1676	1681	rBV3	304501	498742	4.39%	0.277%
15	12.833	1687	1691	1698	rBV3	114915	191923	1.69%	0.106%
16	12.980	1712	1716	1722	rBV3	215949	333555	2.94%	0.185%
17	13.404	1784	1788	1794	rVB	378773	535898	4.72%	0.297%
18	13.463	1795	1798	1800	rBV3	98857	130510	1.15%	0.072%
19	13.504	1802	1805	1811	rVV6	118298	249934	2.20%	0.139%
20	13.727	1839	1843	1845	rBV3	196081	302773	2.67%	0.168%
21	13.816	1854	1858	1863	rVB3	577153	1061530	9.35%	0.589%
22	13.963	1880	1883	1885	rBV2	132167	152382	1.34%	0.085%
23	14.004	1885	1890	1895	rBV	1405449	2119567	18.66%	1.176%
24	14.104	1901	1907	1913	rVB2	616803	1031682	9.08%	0.572%
25	14.233	1925	1929	1931	rBV3	298422	487142	4.29%	0.270%
26	14.269	1931	1935	1940	rVB	1054706	1441982	12.69%	0.800%
27	14.374	1950	1953	1958	rVB	233182	345166	3.04%	0.191%
28	14.557	1981	1984	1992	rVB4	233111	376538	3.31%	0.209%
29	14.627	1994	1996	1998	rBV2	116027	137033	1.21%	0.076%
30	14.663	1999	2002	2008	rVB2	283225	429616	3.78%	0.238%
31	14.798	2021	2025	2028	rBV	389028	518190	4.56%	0.287%
32	14.833	2028	2031	2035	rVB	404404	461931	4.07%	0.256%
33	14.892	2038	2041	2045	rVV	275804	332124	2.92%	0.184%
34	15.051	2066	2068	2075	rBV7	130326	242201	2.13%	0.134%
35	15.398	2123	2127	2132	rVB2	323745	482472	4.25%	0.268%
36	15.521	2143	2148	2154	rBV	2509572	3747893	32.99%	2.079%

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If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM082624.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	15.768	2185	2190	2197	rBV	1103604	1949363	17.16%	1.081%
38	16.015	2228	2232	2240	rVB	1448775	1788977	15.75%	0.992%
39	16.127	2246	2251	2255	rVB	2884285	3595499	31.65%	1.994%
40	16.457	2305	2307	2311	rVB	254206	266904	2.35%	0.148%
41	16.563	2322	2325	2328	rBV	186997	235584	2.07%	0.131%
42	16.610	2330	2333	2339	rVB	391928	623462	5.49%	0.346%
43	16.698	2344	2348	2351	rBV	332992	441402	3.89%	0.245%
44	16.774	2356	2361	2370	rVB	1620642	2360250	20.78%	1.309%
45	17.074	2409	2412	2420	rVB2	296815	456948	4.02%	0.253%
46	17.392	2462	2466	2472	rVB	1356266	1735219	15.28%	0.962%
47	17.457	2474	2477	2488	rVB3	377692	678080	5.97%	0.376%
48	17.610	2499	2503	2507	rVB	1966297	2244309	19.76%	1.245%
49	17.692	2512	2517	2519	rBV	4081004	5753902	50.65%	3.191%
50	17.715	2519	2521	2527	rVB	3821753	4588403	40.39%	2.545%
51	17.980	2563	2566	2576	rVB	477384	763324	6.72%	0.423%
52	18.274	2613	2616	2620	rVB3	158983	198530	1.75%	0.110%
53	18.527	2655	2659	2663	rBV2	305434	481811	4.24%	0.267%
54	18.574	2663	2667	2676	rVB	2318102	3576102	31.48%	1.983%
55	18.792	2700	2704	2710	rVB	1482600	1891469	16.65%	1.049%
56	18.856	2711	2715	2718	rBV	735176	996255	8.77%	0.553%
57	18.886	2718	2720	2726	rVB	592485	750268	6.60%	0.416%
58	18.986	2732	2737	2739	rBV	2318924	2984966	26.28%	1.656%
59	19.015	2739	2742	2744	rVV	3024293	4140791	36.45%	2.297%
60	19.039	2744	2746	2753	rVB	5166291	6205320	54.63%	3.442%
61	19.174	2765	2769	2776	rBV3	411541	835744	7.36%	0.464%
62	19.233	2776	2779	2783	rVV	819734	1105555	9.73%	0.613%
63	19.274	2783	2786	2792	rVB2	964752	1440790	12.68%	0.799%
64	19.439	2809	2814	2819	rBV	5712821	7194931	63.34%	3.990%
65	19.480	2819	2821	2826	rVB2	356475	387763	3.41%	0.215%
66	19.739	2862	2865	2867	rBV	337315	401740	3.54%	0.223%
67	19.774	2867	2871	2877	rVB	1274856	1733717	15.26%	0.962%
68	19.956	2898	2902	2910	rBV	1699453	2142285	18.86%	1.188%
69	20.051	2916	2918	2921	rBV2	107553	127501	1.12%	0.071%
70	20.127	2926	2931	2934	rBV	2820896	3711709	32.68%	2.059%
71	20.162	2934	2937	2941	rVV	5388836	5893228	51.88%	3.268%
72	20.233	2947	2949	2953	rVB	496161	518523	4.56%	0.288%
73	20.280	2953	2957	2961	rVV2	1780703	2301957	20.27%	1.277%
74	20.321	2961	2964	2969	rVV2	645938	975921	8.59%	0.541%
75	20.368	2969	2972	2982	rVB	655318	868961	7.65%	0.482%
76	20.574	3004	3007	3010	rVB	263554	258324	2.27%	0.143%

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 Smoothing : ON Filtering: 5
 Sampling : 1 Min Area: 3 % of largest Peak
 Start Thrs: 0.2 Max Peaks: 100
 Stop Thrs : 0 Peak Location: TOP

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77	20.745	3032	3036	3047	rBV	2040109	2845778	25.05%	1.578%
78	20.956	3066	3072	3076	rBV2	2012760	3891686	34.26%	2.158%
79	21.021	3079	3083	3089	rVB	1690495	2370241	20.87%	1.315%
80	21.127	3096	3101	3103	rBV	2287317	3041760	26.78%	1.687%
81	21.156	3103	3106	3109	rVV	5737844	6776570	59.66%	3.758%
82	21.186	3109	3111	3114	rVV	942847	1152432	10.15%	0.639%
83	21.221	3114	3117	3122	rVB	1556816	1877984	16.53%	1.042%
84	21.280	3122	3127	3129	rBV	488978	737652	6.49%	0.409%
85	21.309	3130	3132	3135	rVV	539372	600457	5.29%	0.333%
86	21.362	3138	3141	3150	rVB	619939	913371	8.04%	0.507%
87	21.733	3199	3204	3214	rVB	1476850	2053033	18.07%	1.139%
88	21.815	3215	3218	3223	rVV	266730	361274	3.18%	0.200%
89	22.044	3252	3257	3262	rBV	1207313	1900509	16.73%	1.054%
90	22.292	3289	3299	3305	rBV2	4249520	11359100	100.00%	6.300%
91	22.450	3321	3326	3335	rVB3	1001314	2334679	20.55%	1.295%
92	22.962	3409	3413	3427	rVB	933742	1857622	16.35%	1.030%
93	23.450	3490	3496	3502	rVB	805836	1574139	13.86%	0.873%
94	25.397	3822	3827	3836	rVB2	518219	1343209	11.82%	0.745%
95	25.856	3892	3905	3915	rBV4	2463701	9205392	81.04%	5.105%
96	27.985	4259	4267	4284	rVB5	699360	3027838	26.66%	1.679%
97	28.868	4404	4417	4435	rVB6	1680677	8650743	76.16%	4.798%

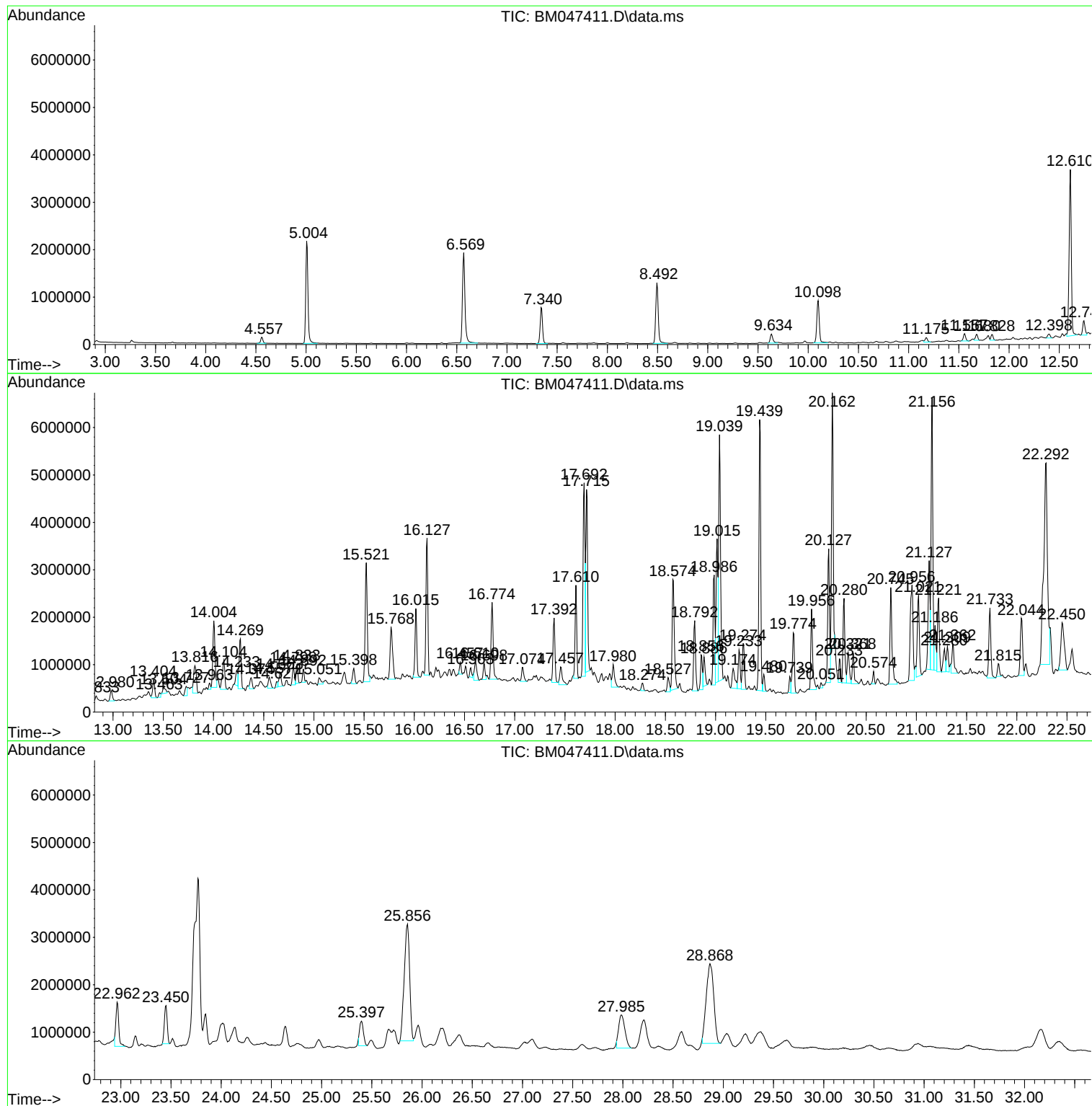
Sum of corrected areas: 180304531

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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM082624.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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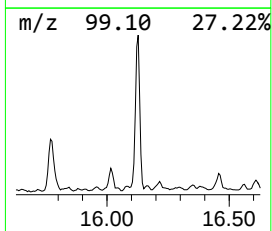
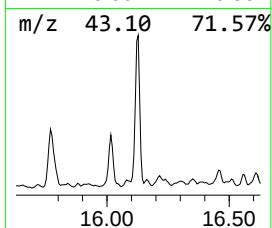
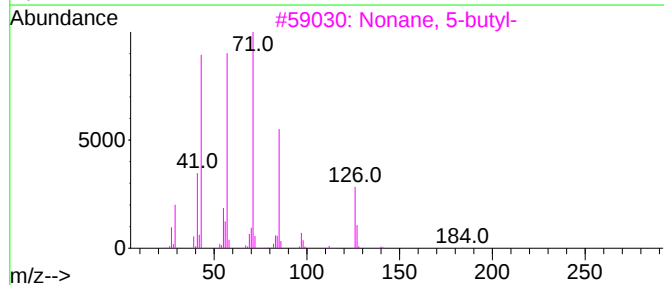
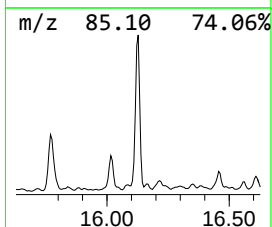
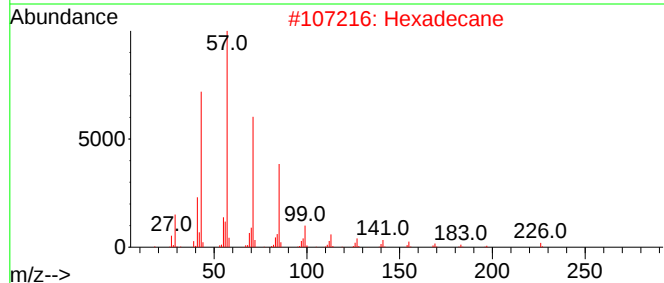
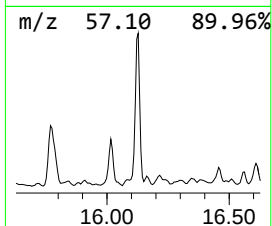
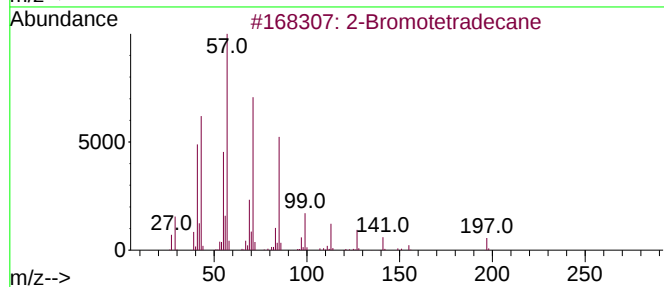
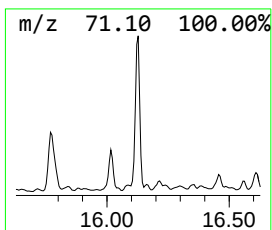
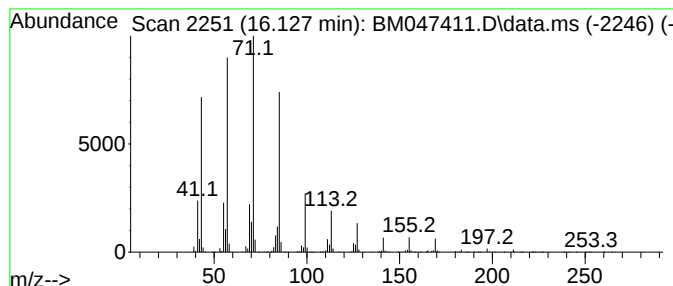
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM082624.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 2-Bromotetradecane Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.127	30.47 ng	3595500	Phenanthrene-d10	16.774

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Bromotetradecane	276	C14H29Br	074036-95-6	90
2			Hexadecane	226	C16H34	000544-76-3	83
3			Nonane, 5-butyl-	184	C13H28	017312-63-9	59
4			Hexane, 2,3,4-trimethyl-	128	C9H20	000921-47-1	58
5			Sulfurous acid, 2-ethylhexyl hex...	278	C14H30O3S	1000309-20-2	53



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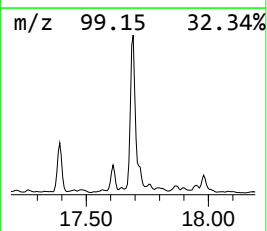
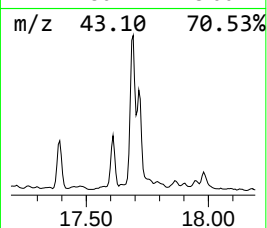
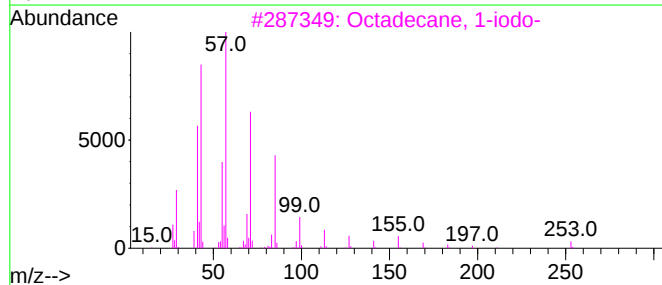
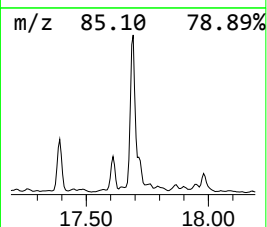
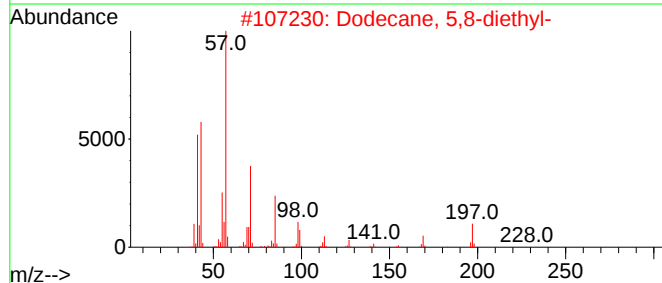
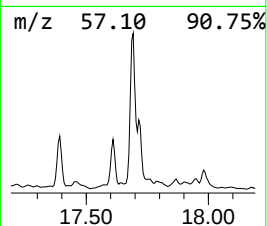
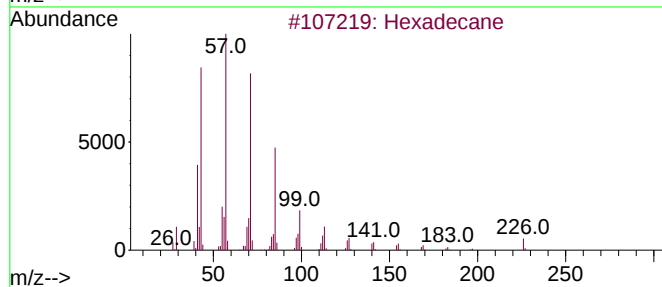
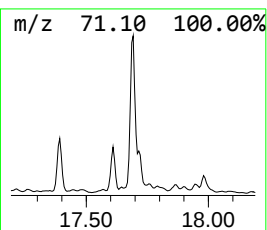
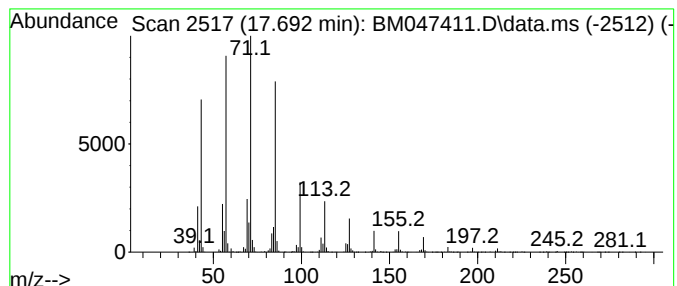
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM082624.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Hexadecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.692	48.76 ng	5753900	Phenanthrene-d10	16.774

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Hexadecane	226	C16H34	000544-76-3	91
2		Dodecane, 5,8-diethyl-	226	C16H34	024251-86-3	87
3		Octadecane, 1-iodo-	380	C18H37I	000629-93-6	80
4		Nonane, 5-butyl-	184	C13H28	017312-63-9	68
5		Dodecane, 2,6,11-trimethyl-	212	C15H32	031295-56-4	55



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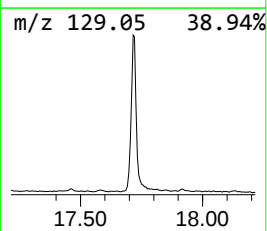
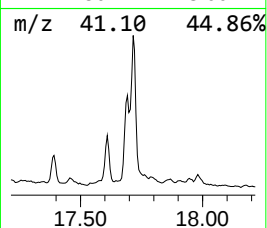
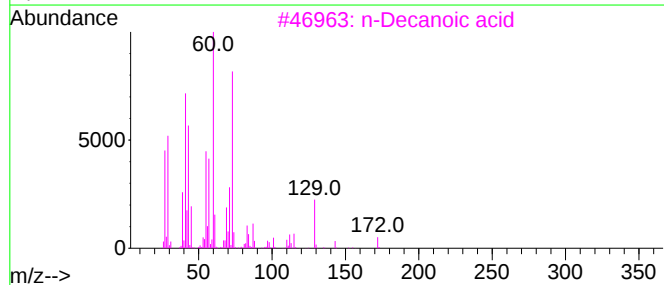
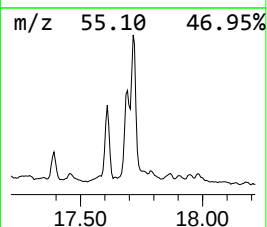
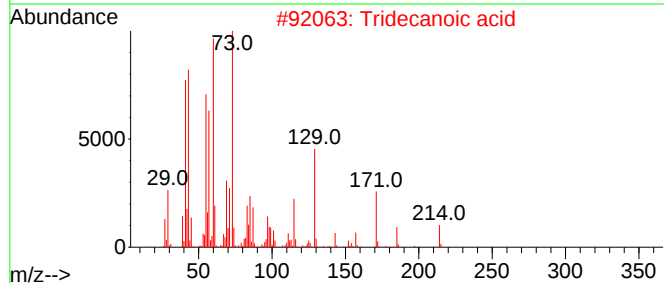
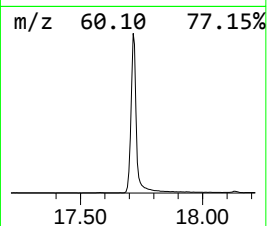
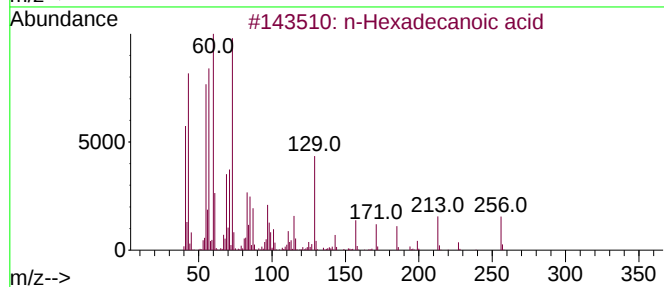
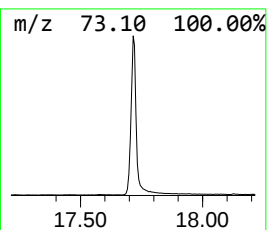
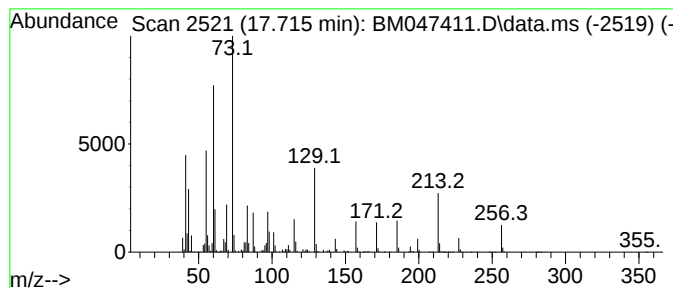
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM082624.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 n-Hexadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.715	38.88 ng	4588400	Phenanthrene-d10	16.774

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	93
2			Tridecanoic acid	214	C13H26O2	000638-53-9	68
3			n-Decanoic acid	172	C10H20O2	000334-48-5	50
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	45
5			Pentadecanoic acid	242	C15H30O2	001002-84-2	42



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Data File : BM047411.D
Acq On : 30 Aug 2024 18:19
Operator : RC/JU
Sample : P3795-03
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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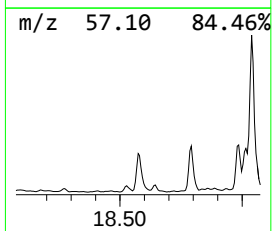
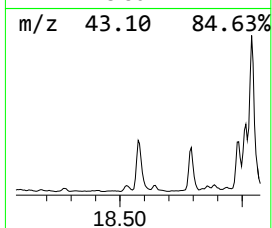
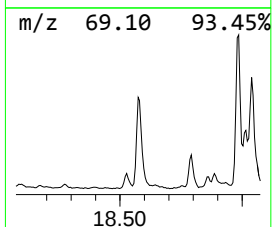
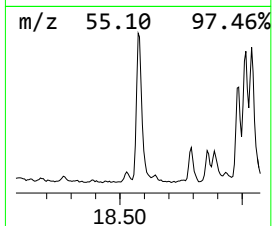
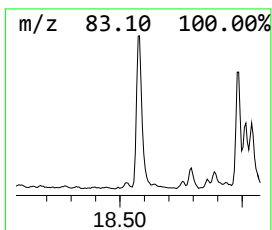
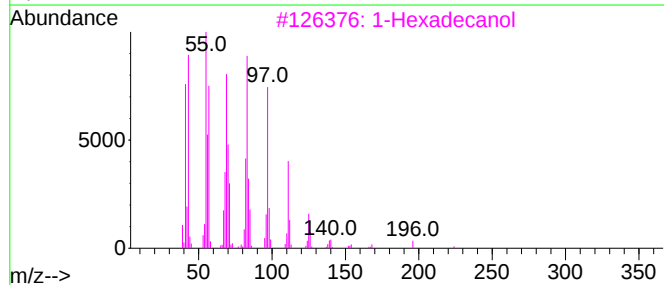
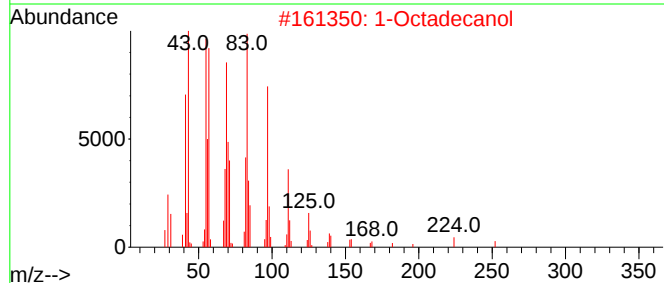
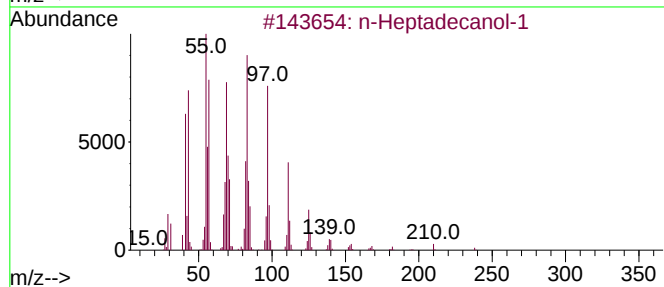
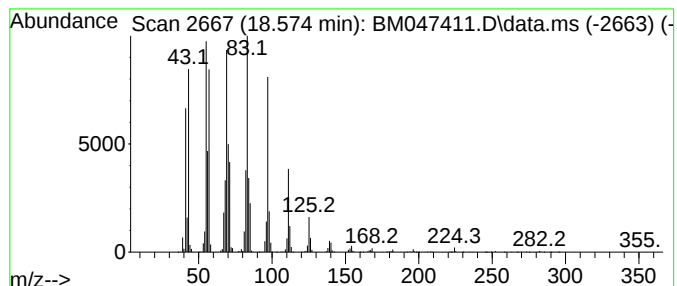
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 n-Heptadecanol-1 Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.574	30.30 ng	3576100	Phenanthrene-d10	16.774

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Heptadecanol-1	256	C17H36O	001454-85-9	95
2		1-Octadecanol	270	C18H38O	000112-92-5	94
3		1-Hexadecanol	242	C16H34O	036653-82-4	93
4		3-Octadecene, (E)-	252	C18H36	007206-19-1	91
5		5-Octadecene, (E)-	252	C18H36	007206-21-5	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM083024\
Data File : BM047411.D
Acq On : 30 Aug 2024 18:19
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Sample : P3795-03
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Instrument :
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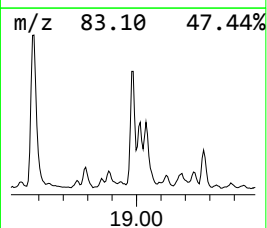
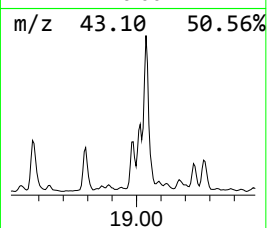
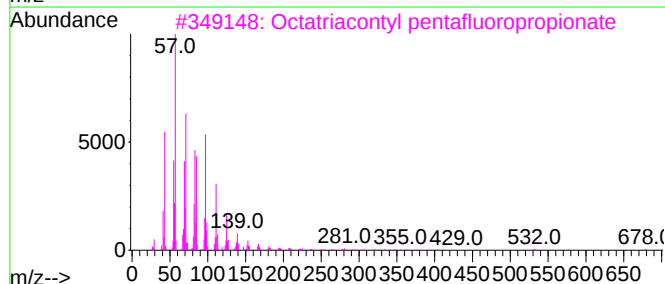
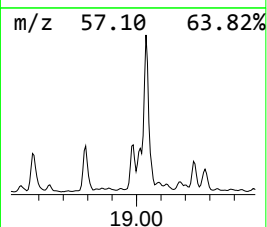
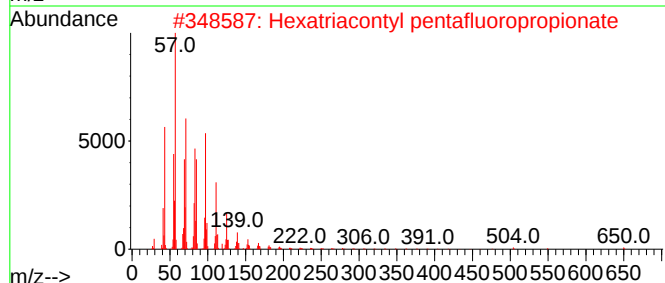
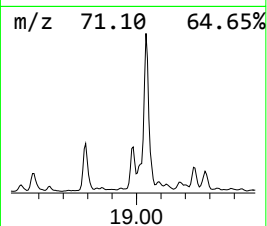
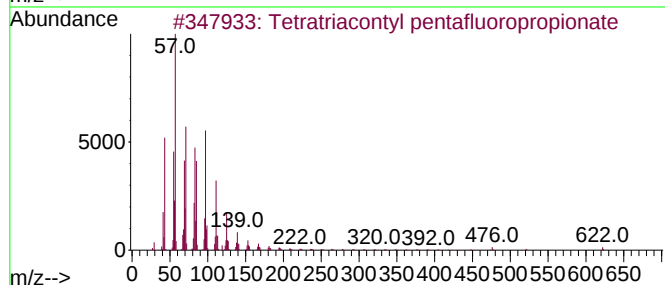
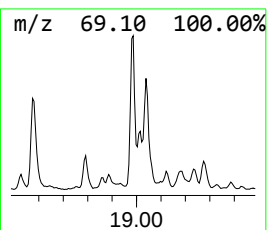
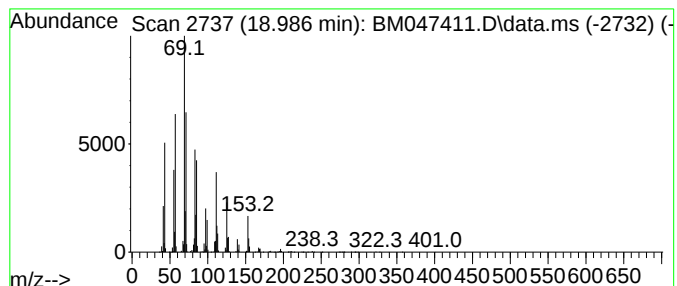
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 unknown18.986 Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.986	25.19 ng	2984970	Chrysene-d12	21.021

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetratriacontyl pentafluoropropi...	641	C37H69F502	1000351-81-5	49
2			Hexatriacontyl pentafluoropropio...	669	C39H73F502	1000351-89-0	49
3			Octatriacontyl pentafluoropropio...	697	C41H77F502	1000351-89-1	49
4			Dotriacontyl trifluoroacetate	562	C34H65F302	1000351-75-4	47
5			Triacacontyl trifluoroacetate	534	C32H61F302	1000351-75-7	47



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM083024\
Data File : BM047411.D
Acq On : 30 Aug 2024 18:19
Operator : RC/JU
Sample : P3795-03
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
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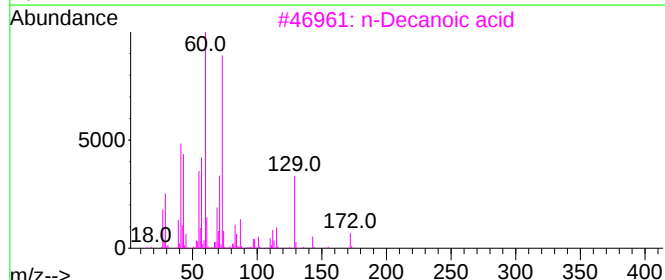
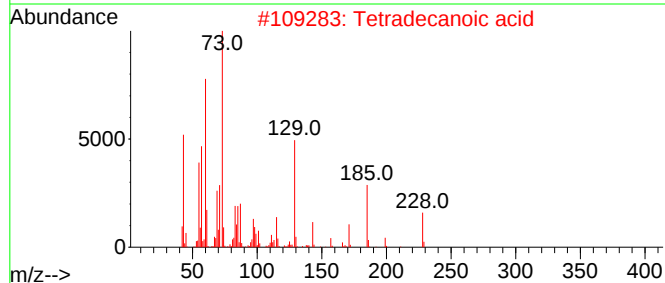
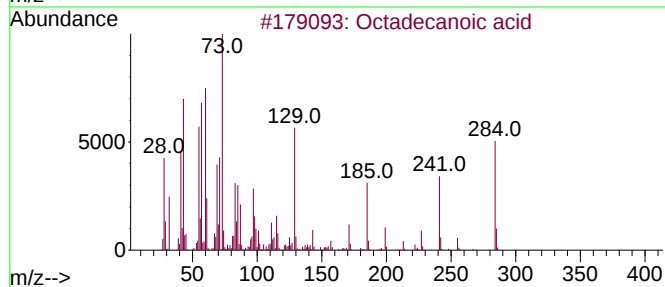
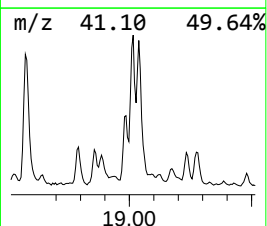
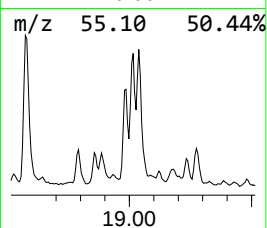
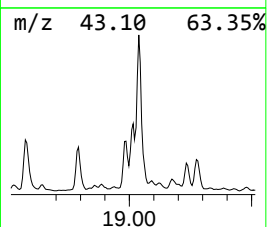
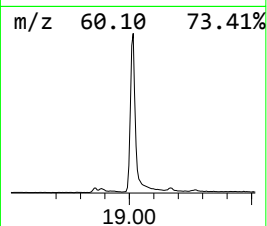
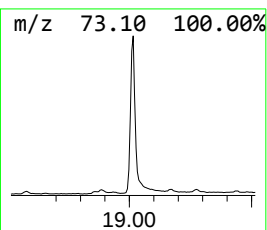
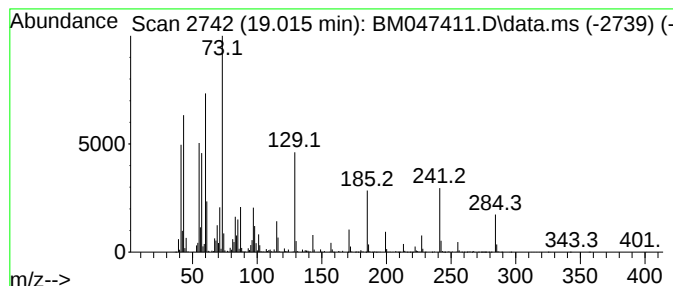
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Octadecanoic acid Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.015	34.94 ng	4140790	Chrysene-d12	21.021

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	93
2			Tetradecanoic acid	228	C14H28O2	000544-63-8	62
3			n-Decanoic acid	172	C10H20O2	000334-48-5	58
4			Tridecanoic acid	214	C13H26O2	000638-53-9	43
5			Pentadecanoic acid	242	C15H30O2	001002-84-2	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM083024\
Data File : BM047411.D
Acq On : 30 Aug 2024 18:19
Operator : RC/JU
Sample : P3795-03
Misc :
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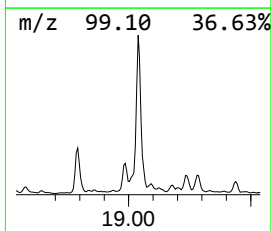
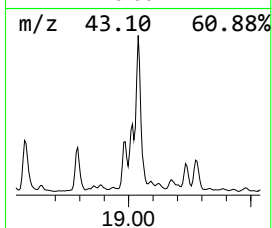
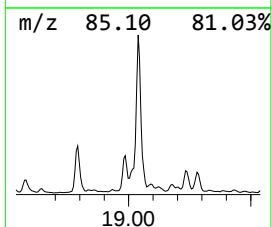
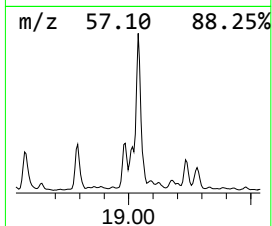
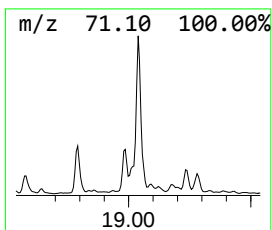
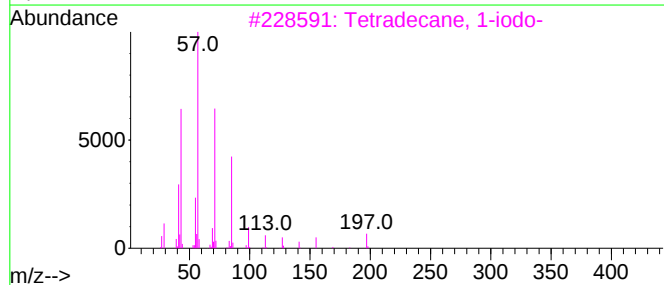
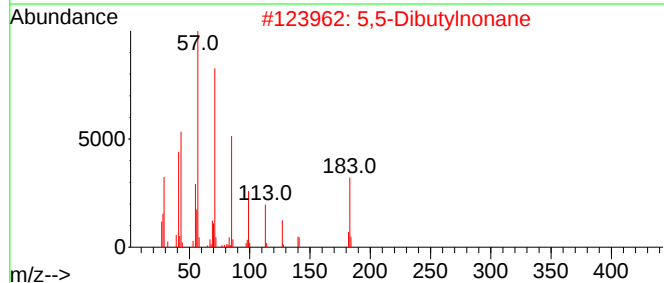
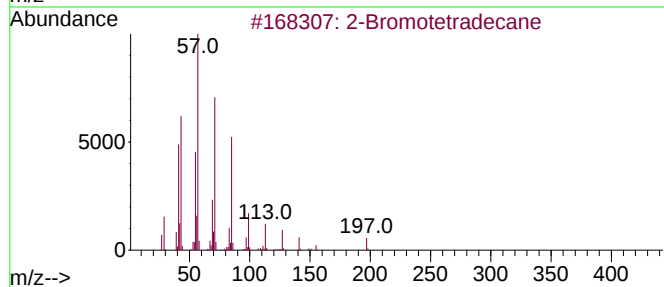
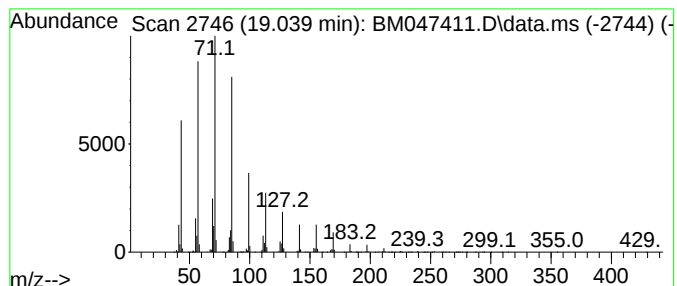
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 5,5-Dibutylnonane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD		R.T.	
19.039	52.36 ng	6205320	Chrysene-d12		21.021	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	2-Bromotetradecane		276	C14H29Br	074036-95-6	83
2	5,5-Dibutylnonane		240	C17H36	006008-17-9	64
3	Tetradecane, 1-iodo-		324	C14H29I	019218-94-1	64
4	Decane, 3,8-dimethyl-		170	C12H26	017312-55-9	53
5	Hexadecane, 2-methyl-		240	C17H36	001560-92-5	50



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM083024\
Data File : BM047411.D
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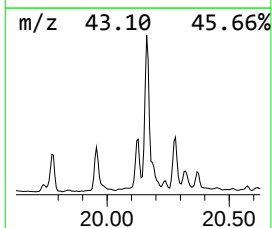
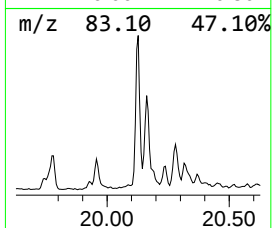
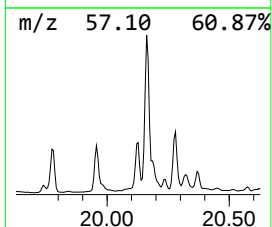
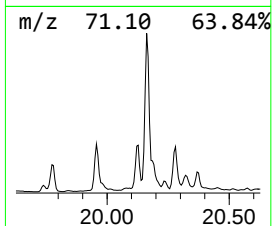
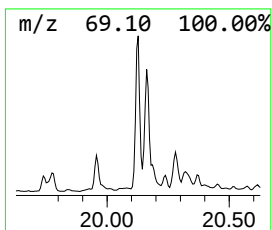
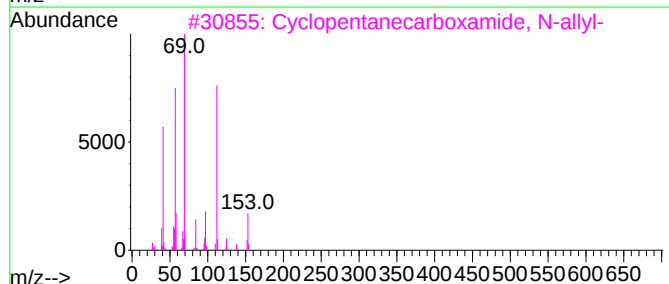
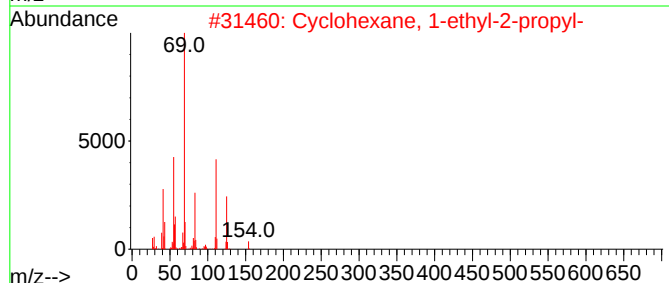
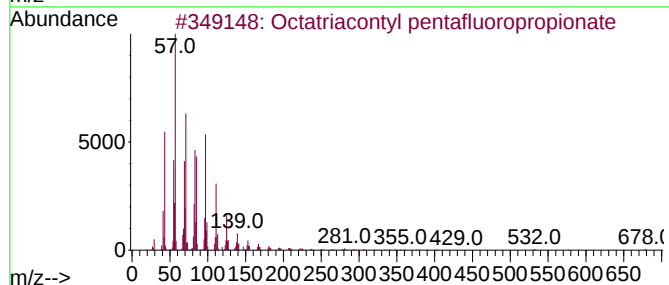
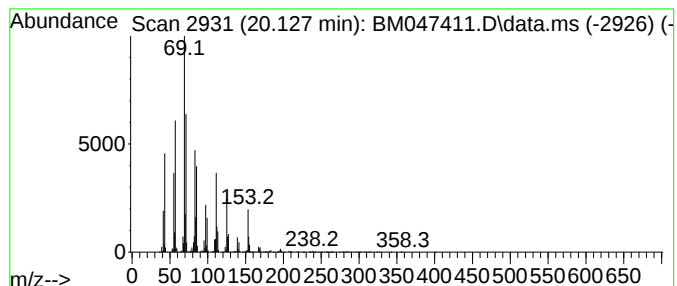
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 8 unknown20.127 Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.	
20.127	31.32 ng	3711710	Chrysene-d12	21.021	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octatriacontyl pentafluoropropio...	697	C41H77F5O2	1000351-89-1	43
2	Cyclohexane, 1-ethyl-2-propyl-	154	C11H22	062238-33-9	35
3	Cyclopentanecarboxamide, N-allyl-	153	C9H15NO	1010340-11-3	30
4	4-Octene, 2,3,6-trimethyl-	154	C11H22	063830-65-9	27
5	Pentyl octadecyl ether	340	C23H48O	1000406-41-9	27



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM083024\
Data File : BM047411.D
Acq On : 30 Aug 2024 18:19
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Sample : P3795-03
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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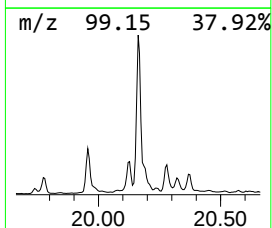
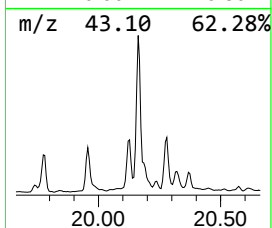
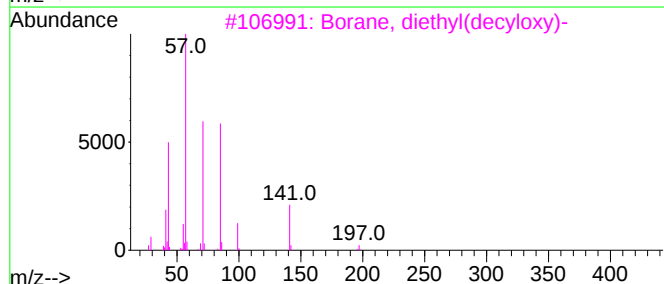
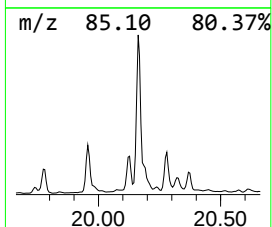
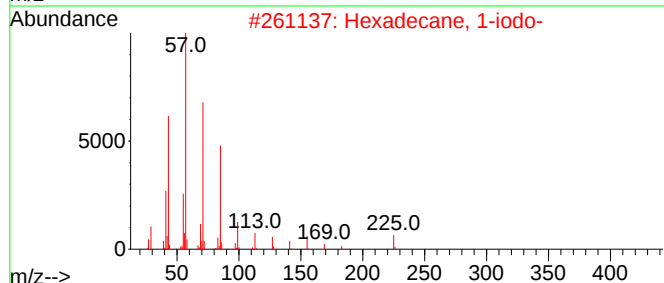
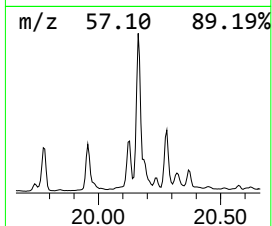
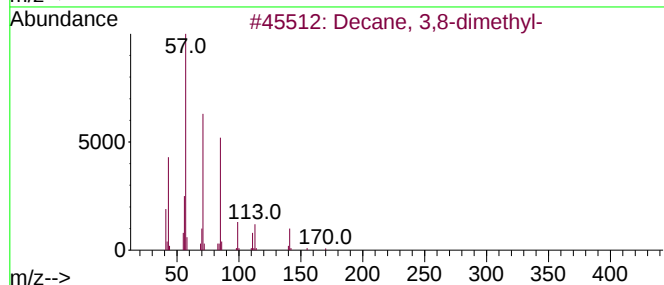
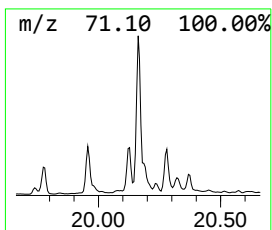
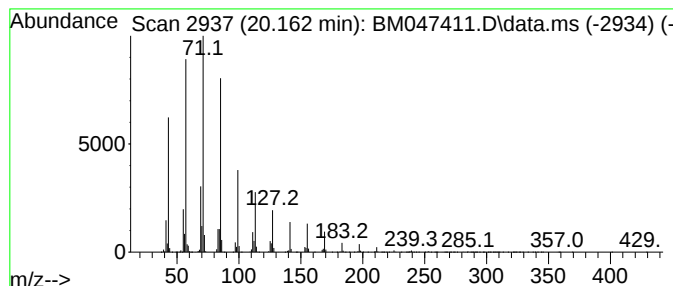
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 9 Decane, 3,8-dimethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.162	49.73 ng	5893230	Chrysene-d12	21.021

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Decane, 3,8-dimethyl-	170	C12H26	017312-55-9	64
2			Hexadecane, 1-iodo-	352	C16H33I	000544-77-4	59
3			Borane, diethyl(decyloxy)-	226	C14H31BO	1000152-34-3	49
4			Hexane, 2,3,4-trimethyl-	128	C9H20	000921-47-1	47
5			Dodecane, 4-methyl-	184	C13H28	006117-97-1	46



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM083024\
Data File : BM047411.D
Acq On : 30 Aug 2024 18:19
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Sample : P3795-03
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ALS Vial : 12 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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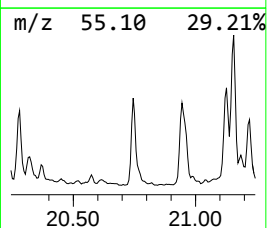
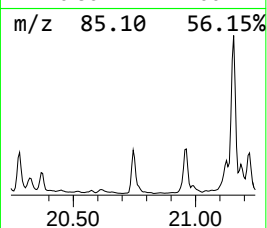
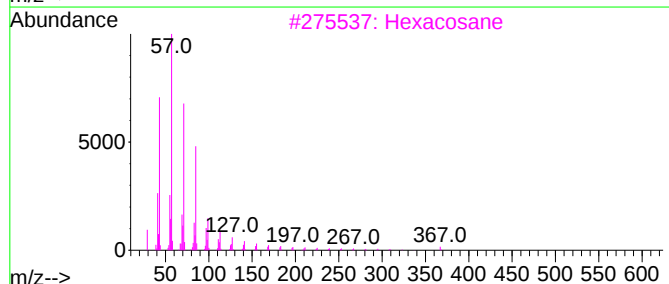
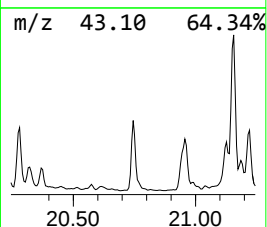
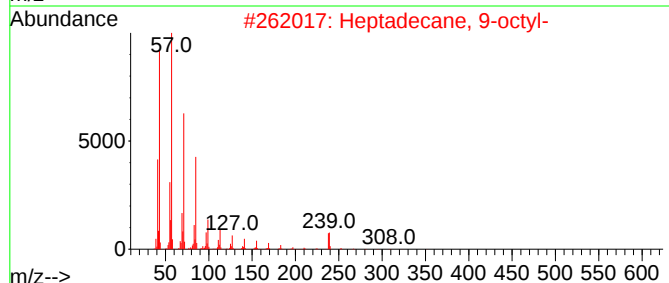
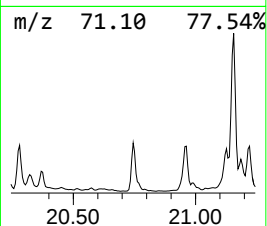
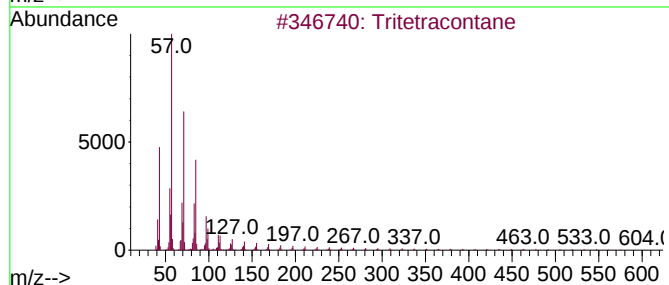
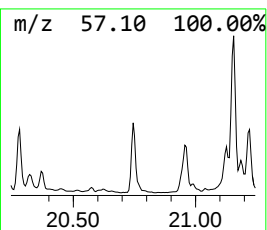
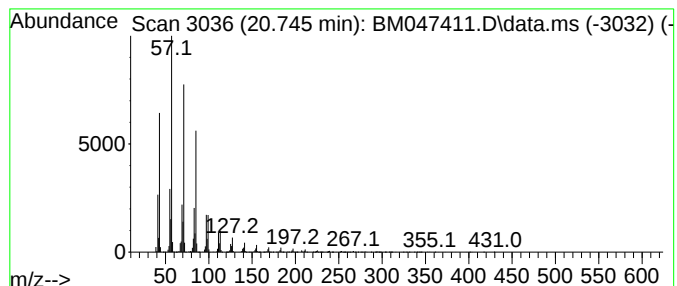
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 10 Tritetracontane Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.745	24.01 ng	2845780	Chrysene-d12	21.021

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Tritetracontane	605	C43H88	007098-21-7	91
2		Heptadecane, 9-octyl-	352	C25H52	007225-64-1	90
3		Hexacosane	366	C26H54	000630-01-3	90
4		Octacosane	394	C28H58	000630-02-4	87
5		Sulfurous acid, dodecyl 2-propyl...	292	C15H32O3S	1000309-12-3	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM083024\
Data File : BM047411.D
Acq On : 30 Aug 2024 18:19
Operator : RC/JU
Sample : P3795-03
Misc :
ALS Vial : 12 Sample Multiplier: 1

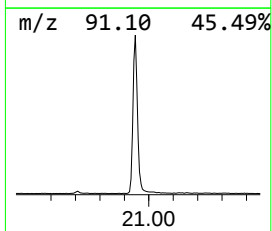
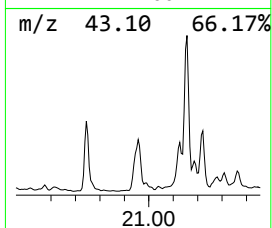
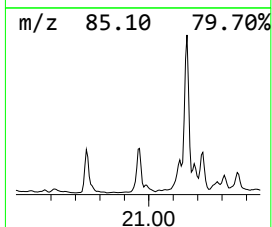
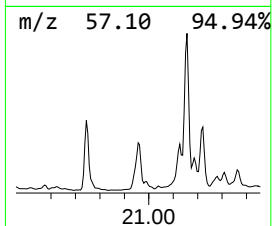
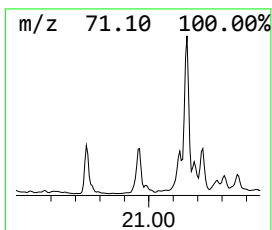
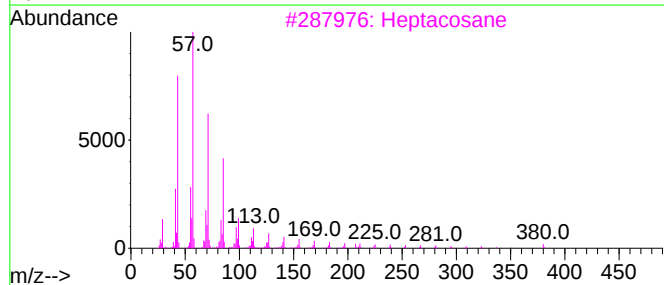
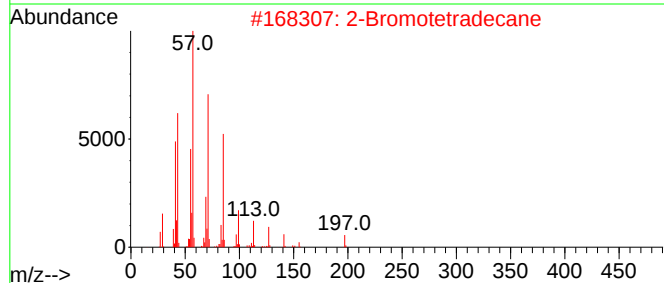
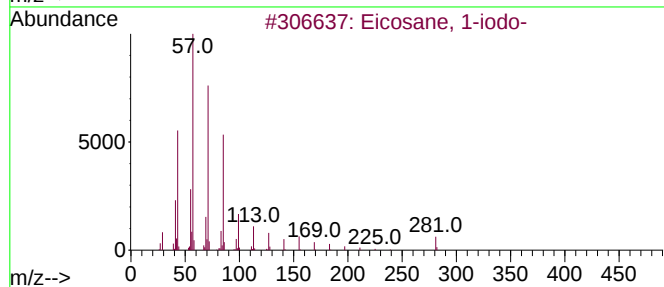
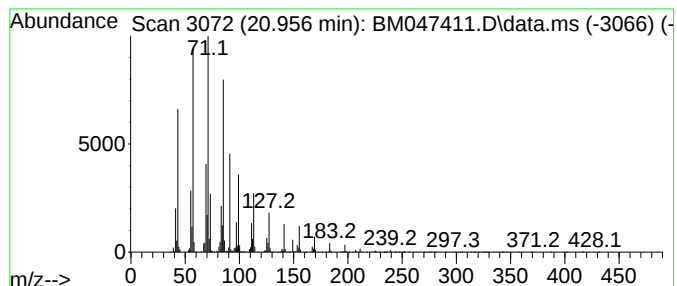
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 11 Eicosane, 1-iodo- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.	
20.956	32.84 ng	3891690	Chrysene-d12	21.021	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane, 1-iodo-	408	C20H41I	1000406-31-8	80
2	2-Bromotetradecane	276	C14H29Br	074036-95-6	80
3	Heptacosane	380	C27H56	000593-49-7	80
4	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	80
5	Hexacosane	366	C26H54	000630-01-3	78



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM083024\
Data File : BM047411.D
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Sample : P3795-03
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Instrument :
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ClientSampleId :
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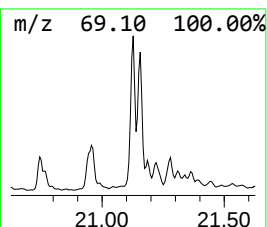
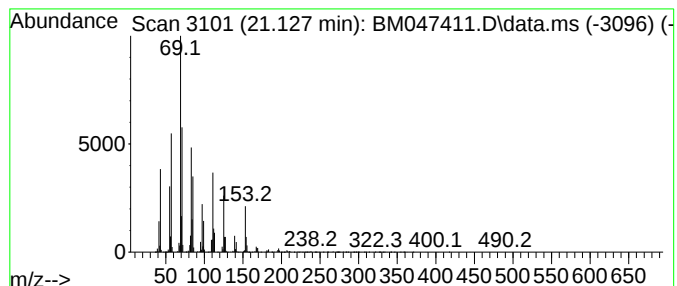
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 12 unknown21.127 Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.127	25.67 ng	3041760	Chrysene-d12	21.021

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octacosyl trifluoroacetate	506	C30H57F3O2	1000351-74-9	46
2			Tetratriacontyl heptafluorobutyrate	691	C38H69F7O2	1000351-84-1	43
3			Tetratriacontyl pentafluoropropi...	641	C37H69F5O2	1000351-81-5	43
4			Hexatriacontyl pentafluoropropio...	669	C39H73F5O2	1000351-89-0	43
5			Tetracosyl heptafluorobutyrate	550	C28H49F7O2	1000351-83-7	43



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM083024\
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Sample : P3795-03
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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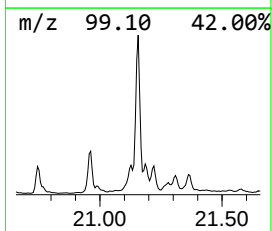
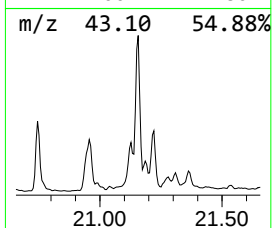
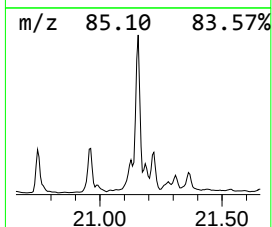
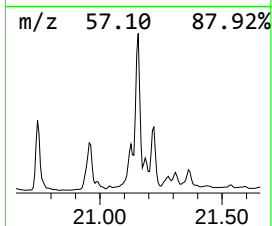
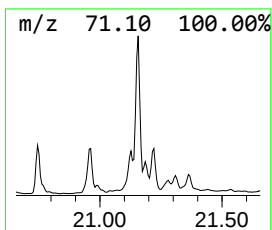
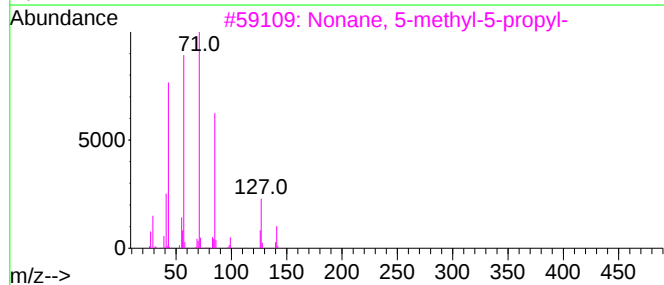
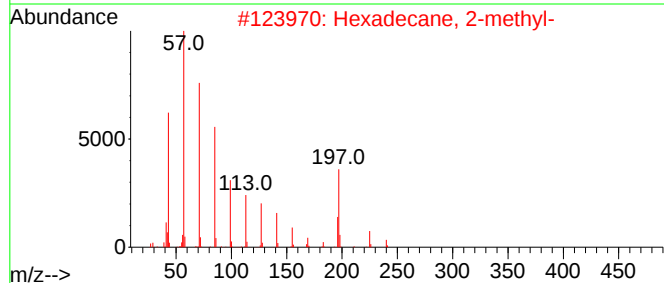
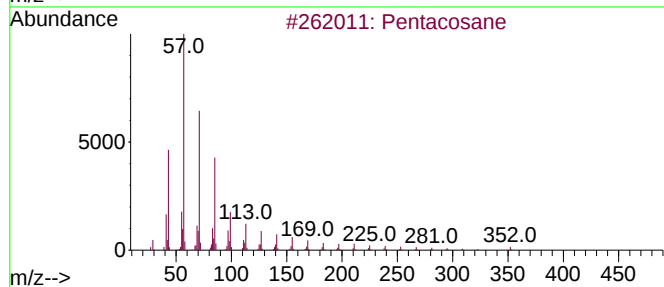
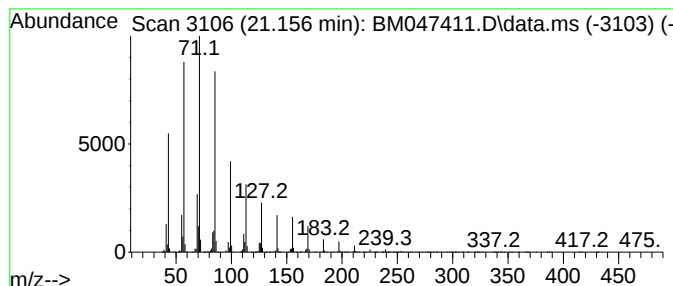
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 13 Pentacosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.156	57.18 ng	6776570	Chrysene-d12	21.021

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentacosane	352	C25H52	000629-99-2	83
2			Hexadecane, 2-methyl-	240	C17H36	001560-92-5	72
3			Nonane, 5-methyl-5-propyl-	184	C13H28	017312-75-3	53
4			Decane, 3,8-dimethyl-	170	C12H26	017312-55-9	50
5			Nonane, 1-iodo-	254	C9H19I	004282-42-2	50



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM083024\
Data File : BM047411.D
Acq On : 30 Aug 2024 18:19
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Sample : P3795-03
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Instrument :
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ClientSampleId :
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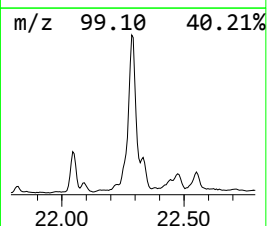
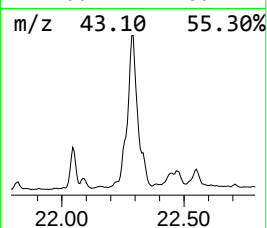
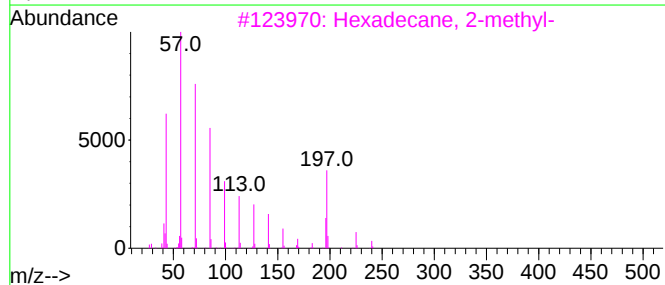
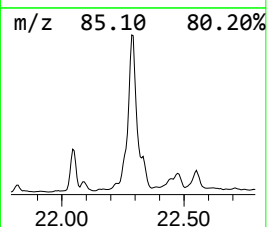
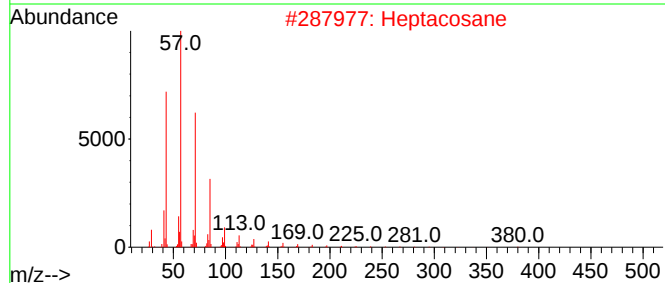
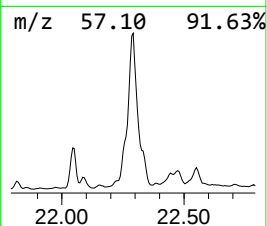
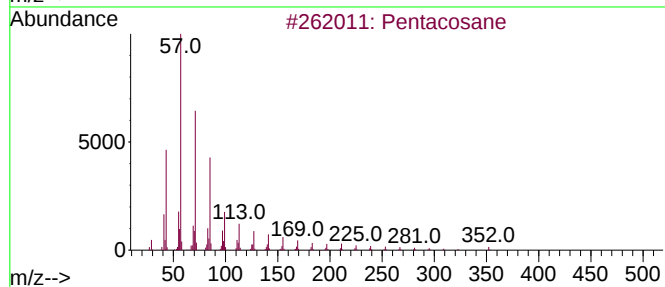
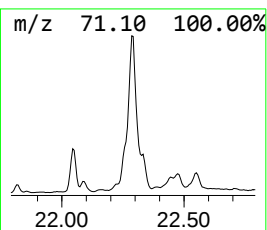
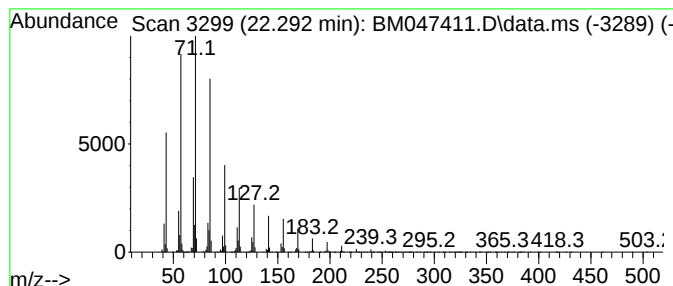
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 14 Heptacosane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.292	95.85 ng	11359100	Chrysene-d12	21.021

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Pentacosane	352	C25H52	000629-99-2	90
2		Heptacosane	380	C27H56	000593-49-7	86
3		Hexadecane, 2-methyl-	240	C17H36	001560-92-5	64
4		Undecane, 2-methyl-	170	C12H26	007045-71-8	59
5		Tridecane, 7-propyl-	226	C16H34	055045-09-5	58



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM083024\
Data File : BM047411.D
Acq On : 30 Aug 2024 18:19
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Sample : P3795-03
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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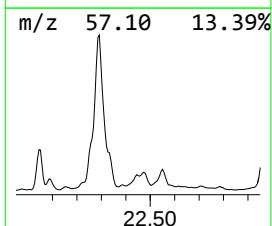
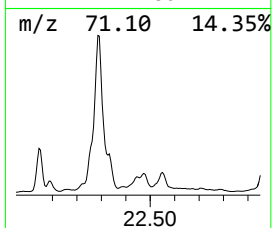
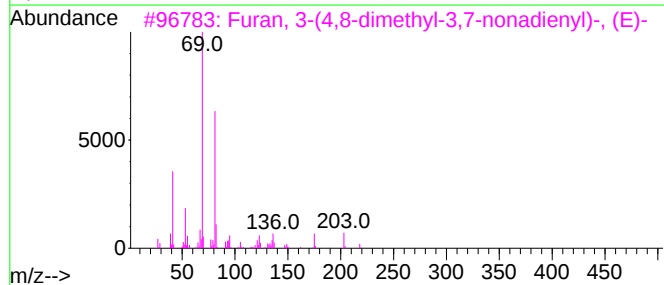
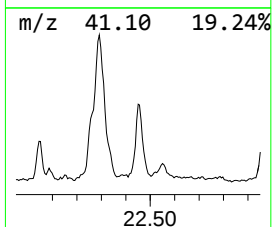
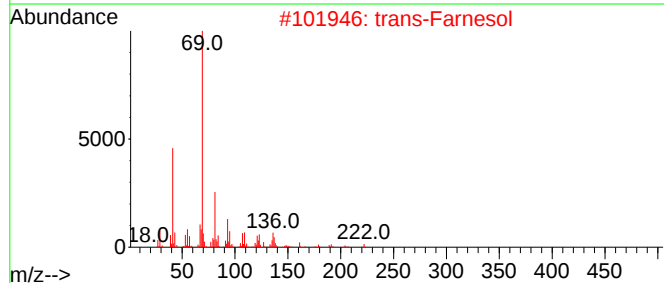
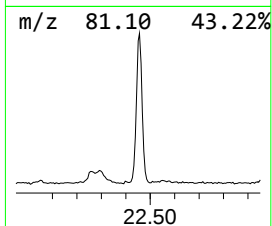
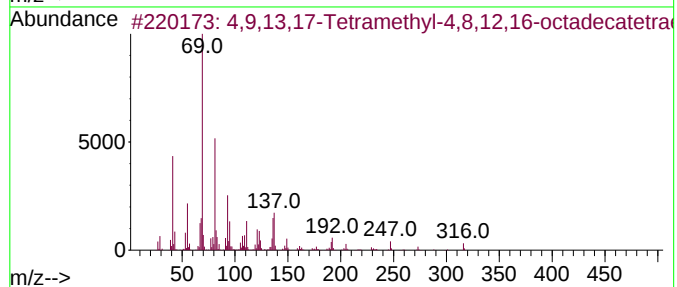
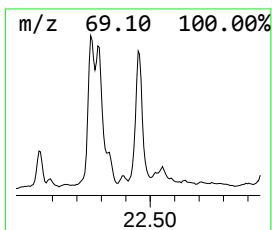
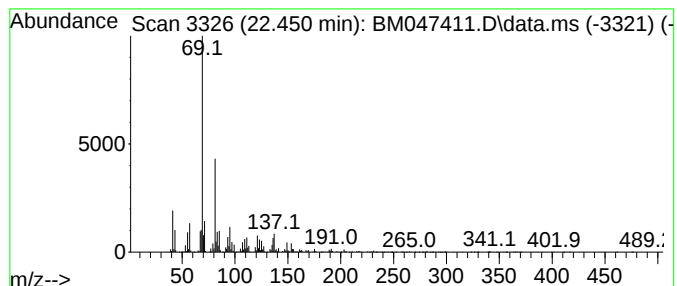
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 15 4,9,13,17-Tetramethyl-4,8,1... Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.450	29.66 ng	2334680	Perylene-d12	23.721

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	4,9,13,17-Tetramethyl-4,8,12,16-...	316	C22H36O	056882-09-8	64		
2	trans-Farnesol	222	C15H26O	000106-28-5	64		
3	Furan, 3-(4,8-dimethyl-3,7-nonadecyl)-	218	C15H22O	023262-34-2	59		
4	1H-Imidazole, 1-(1-oxooctadecyl)-	334	C21H38N2O	017450-32-7	59		
5	Succinic acid, 3-methylbut-2-en-...	316	C15H15F3O4	1000390-75-8	53		



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM083024\
Data File : BM047411.D
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Instrument :
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ClientSampleId :
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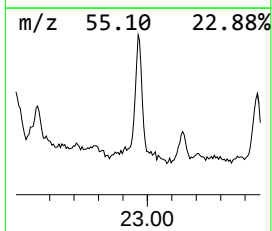
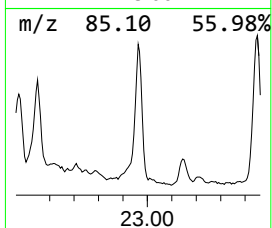
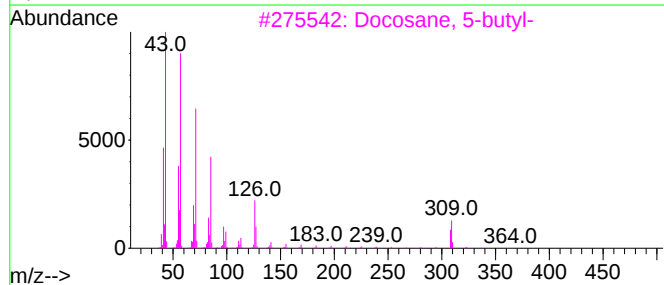
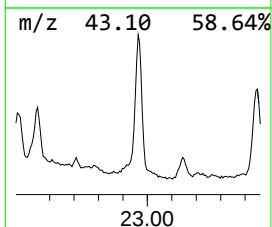
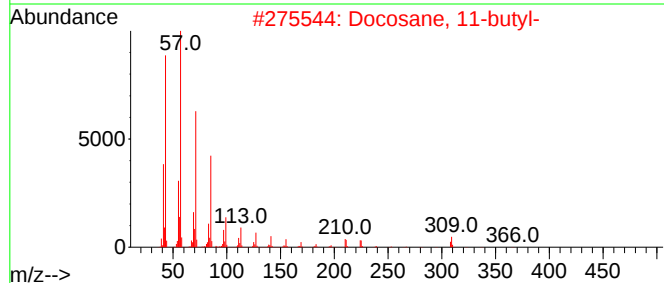
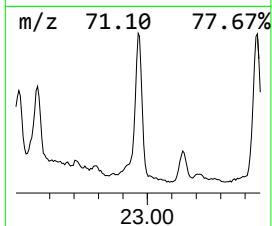
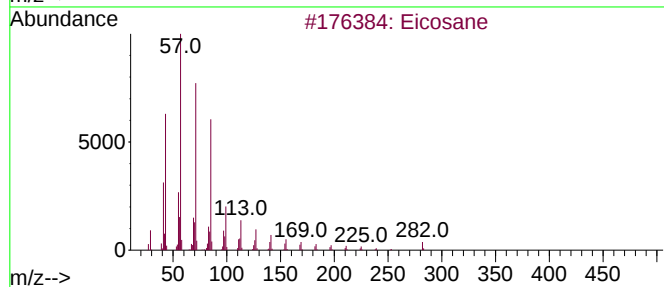
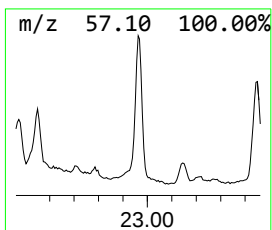
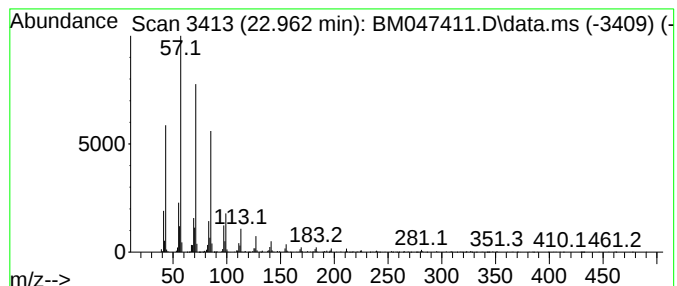
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 16 Eicosane Concentration Rank 19

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.962	23.60 ng	1857620	Perylene-d12	23.721

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane		282	C20H42	000112-95-8	95
2	Docosane, 11-butyl-		366	C26H54	013475-76-8	94
3	Docosane, 5-butyl-		366	C26H54	055282-16-1	91
4	Docosane, 9-butyl-		366	C26H54	055282-14-9	91
5	Heneicosane		296	C21H44	000629-94-7	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM083024\
Data File : BM047411.D
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ALS Vial : 12 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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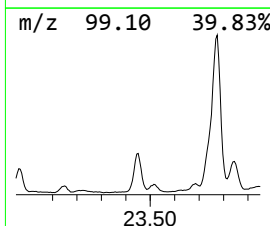
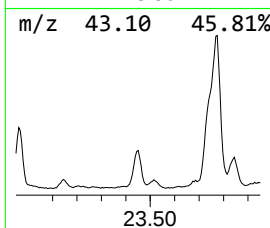
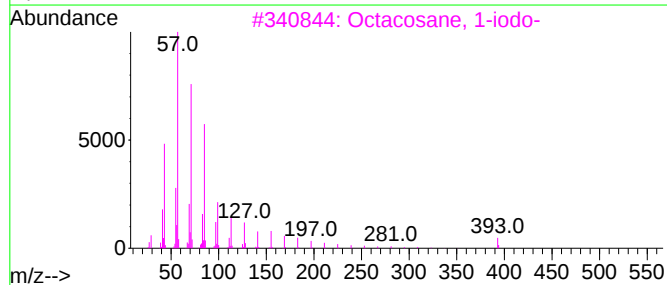
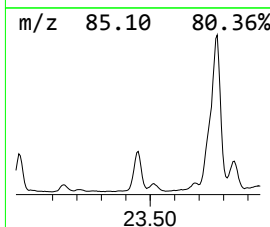
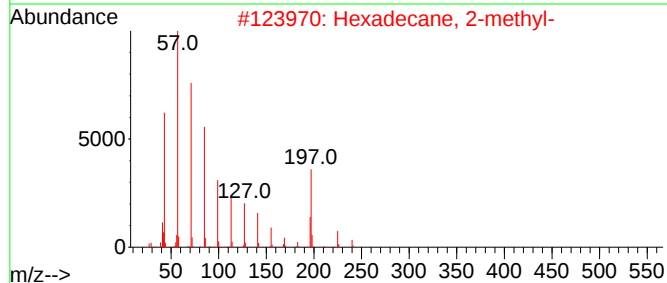
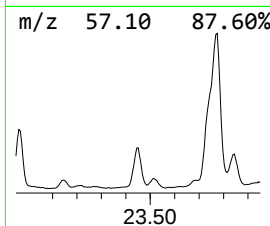
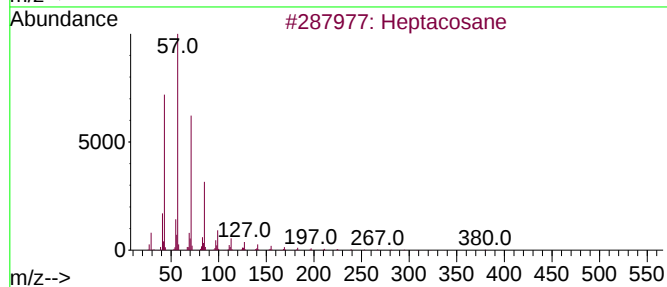
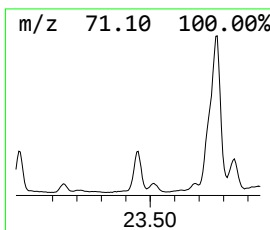
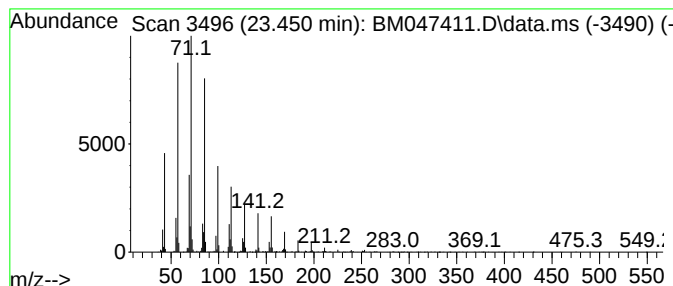
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 17 Hexadecane, 2-methyl- Concentration Rank 20

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.450	20.00 ng	1574140	Perylene-d12	23.721

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Heptacosane	380	C27H56	000593-49-7	91
2		Hexadecane, 2-methyl-	240	C17H36	001560-92-5	86
3		Octacosane, 1-iodo-	520	C28H57I	1000406-32-2	83
4		Pentacosane	352	C25H52	000629-99-2	80
5		Eicosane, 1-iodo-	408	C20H41I	1000406-31-8	72



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM083024\
Data File : BM047411.D
Acq On : 30 Aug 2024 18:19
Operator : RC/JU
Sample : P3795-03
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
239

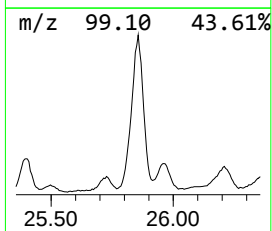
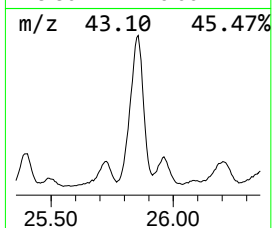
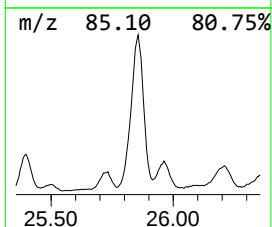
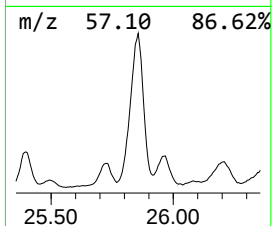
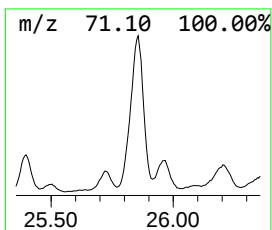
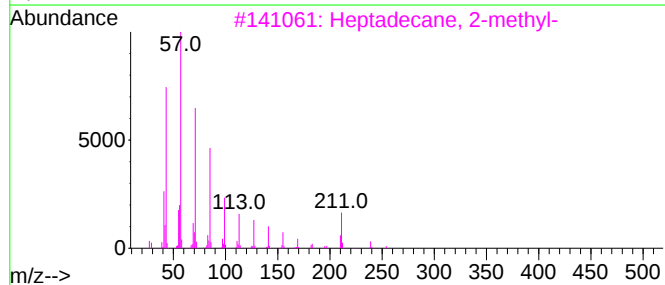
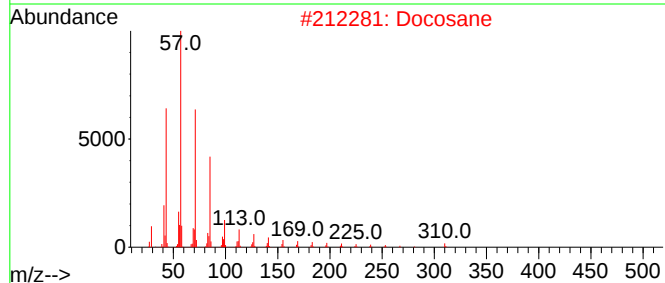
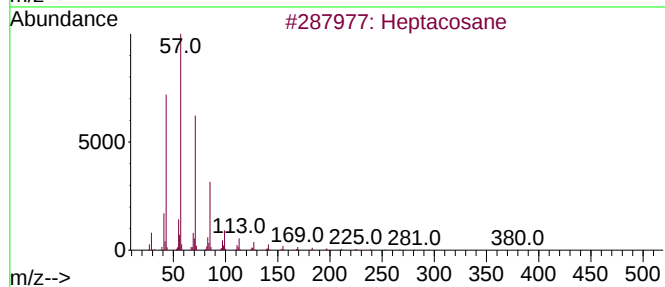
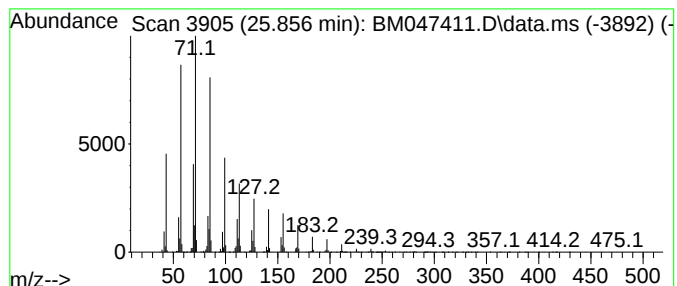
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 18 Docosane Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
25.856	116.96 ng	9205390	Perylene-d12	23.721

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Heptacosane	380	C27H56	000593-49-7	90
2		Docosane	310	C22H46	000629-97-0	86
3		Heptadecane, 2-methyl-	254	C18H38	001560-89-0	78
4		Hexadecane, 2-methyl-	240	C17H36	001560-92-5	78
5		Eicosane, 1-iodo-	408	C20H41I	1000406-31-8	59



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM083024\
Data File : BM047411.D
Acq On : 30 Aug 2024 18:19
Operator : RC/JU
Sample : P3795-03
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
239

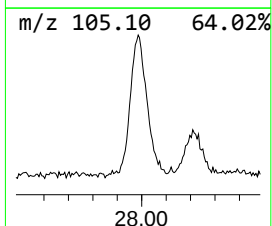
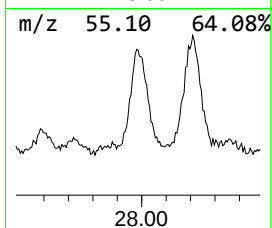
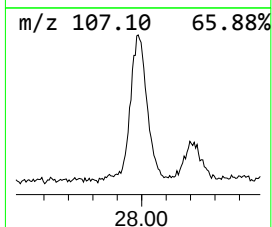
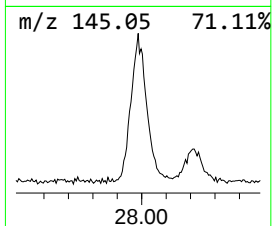
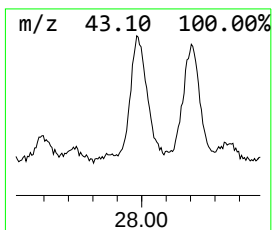
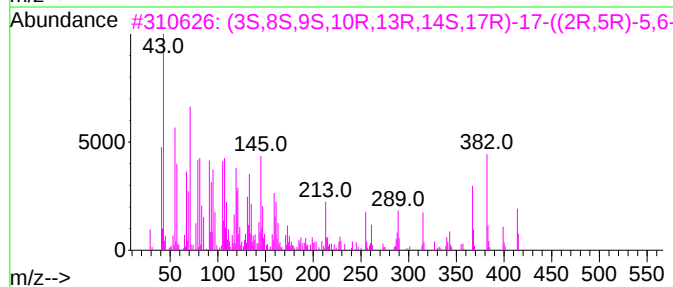
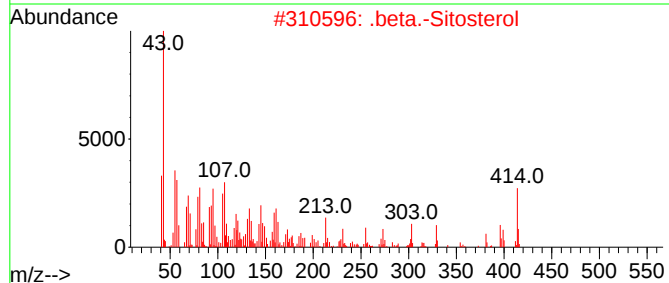
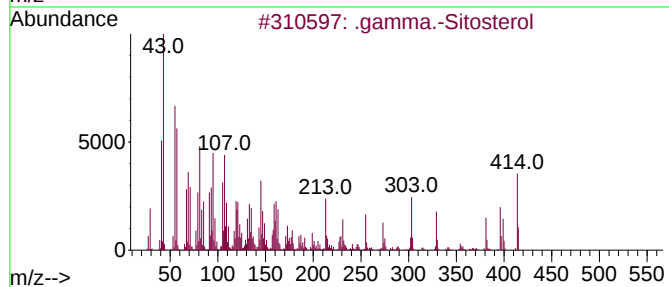
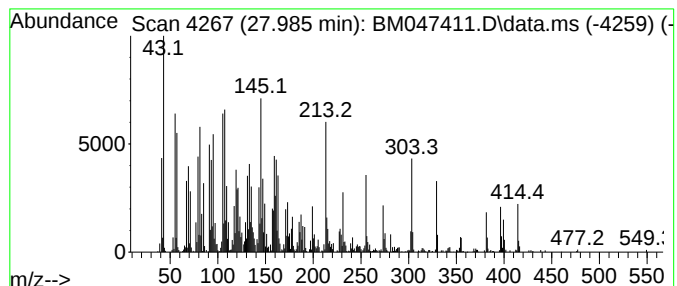
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 19 .gamma.-Sitosterol Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
27.985	38.47 ng	3027840	Perylene-d12	23.721

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		.gamma.-Sitosterol	414	C29H50O	000083-47-6	98
2		.beta.-Sitosterol	414	C29H50O	000083-46-5	78
3		(3S,8S,9S,10R,13R,14S,17R)-17-((...)	414	C29H50O	029365-29-5	64
4		Ergost-5-en-3-ol, (3.beta.)-	400	C28H48O	004651-51-8	49
5		(3S,8S,9S,10R,13R,14S,17R)-17-((...)	428	C30H52O	020194-50-7	25



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM083024\
Data File : BM047411.D
Acq On : 30 Aug 2024 18:19
Operator : RC/JU
Sample : P3795-03
Misc :
ALS Vial : 12 Sample Multiplier: 1

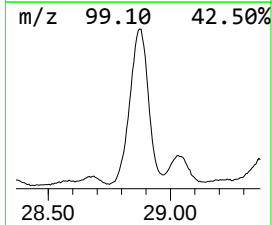
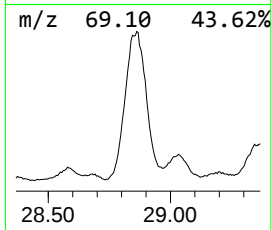
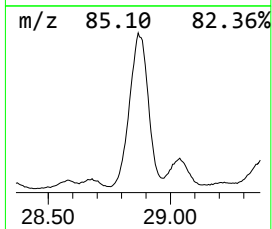
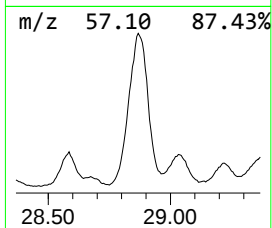
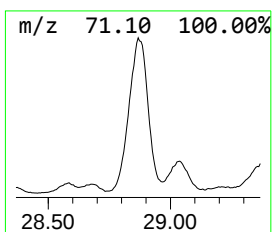
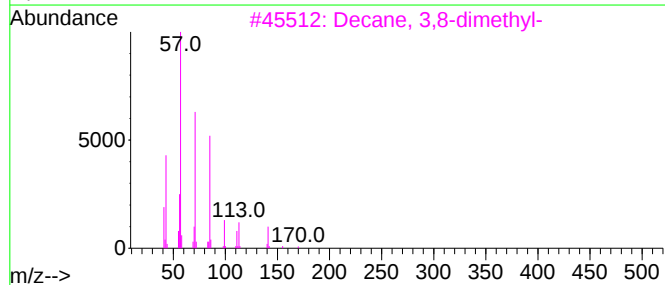
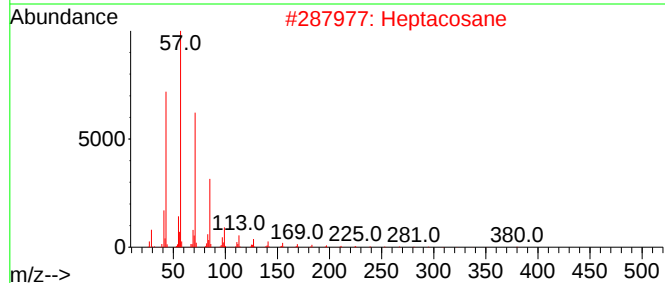
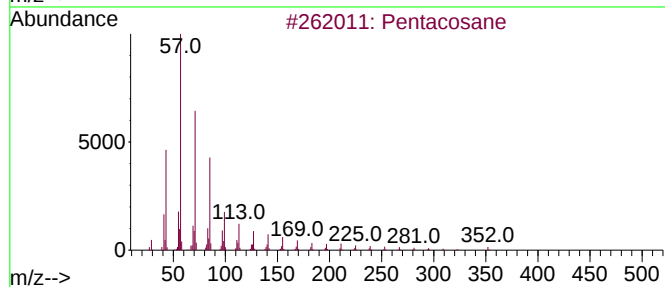
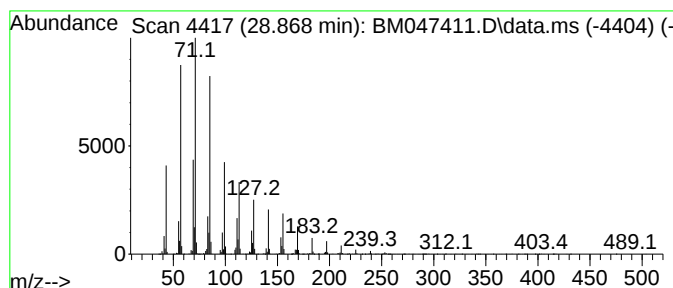
Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM082624.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 20 Octadecane, 1-iodo- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
28.868	109.91 ng	8650740	Perylene-d12	23.721	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentacosane	352	C25H52	000629-99-2	90
2	Heptacosane	380	C27H56	000593-49-7	86
3	Decane, 3,8-dimethyl-	170	C12H26	017312-55-9	76
4	Octadecane, 1-iodo-	380	C18H37I	000629-93-6	72
5	Hexadecane, 1-iodo-	352	C16H33I	000544-77-4	43



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM083024\
Data File : BM047411.D
Acq On : 30 Aug 2024 18:19
Operator : RC/JU
Sample : P3795-03
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
239

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM082624.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
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Hexadecane	17.692	48.8	ng	5753900	4	16.774	2360250	20.0
n-Hexadecanoic ...	17.715	38.9	ng	4588400	4	16.774	2360250	20.0
n-Heptadecanol-1	18.574	30.3	ng	3576100	4	16.774	2360250	20.0
unknown18.986	18.986	25.2	ng	2984970	5	21.021	2370240	20.0
Octadecanoic acid	19.015	34.9	ng	4140790	5	21.021	2370240	20.0
5,5-Dibutylnonane	19.039	52.4	ng	6205320	5	21.021	2370240	20.0
unknown20.127	20.127	31.3	ng	3711710	5	21.021	2370240	20.0
Decane, 3,8-dim...	20.162	49.7	ng	5893230	5	21.021	2370240	20.0
Tritetracontane	20.745	24.0	ng	2845780	5	21.021	2370240	20.0
Eicosane, 1-iodo-	20.956	32.8	ng	3891690	5	21.021	2370240	20.0
unknown21.127	21.127	25.7	ng	3041760	5	21.021	2370240	20.0
Pentacosane	21.156	57.2	ng	6776570	5	21.021	2370240	20.0
Heptacosane	22.292	95.8	ng	11359100	5	21.021	2370240	20.0
4,9,13,17-Tetra...	22.450	29.7	ng	2334680	6	23.721	1574140	20.0
Eicosane	22.962	23.6	ng	1857620	6	23.721	1574140	20.0
Hexadecane, 2-m...	23.450	20.0	ng	1574140	6	23.721	1574140	20.0
Docosane	25.856	117.0	ng	9205390	6	23.721	1574140	20.0
.gamma.-Sitosterol	27.985	38.5	ng	3027840	6	23.721	1574140	20.0
Octadecane, 1-i...	28.868	109.9	ng	8650740	6	23.721	1574140	20.0