

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082224\
 Data File : BF139117.D
 Acq On : 22 Aug 2024 12:22
 Operator : RC/JU
 Sample : P3641-04
 Misc :
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 S-908-K1-0.5-1.0-081524

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_F\Methods\8270-BF082024.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF139117.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.222	14	22	29	rBV	1074404	1629570	82.13%	5.905%
2	3.052	156	163	172	rVB	20795	37992	1.91%	0.138%
3	5.116	504	514	529	rVB	134777	210255	10.60%	0.762%
4	5.510	575	581	587	rBV	1264137	1682498	84.80%	6.097%
5	6.181	690	695	702	rVB	93473	115236	5.81%	0.418%
6	6.516	745	752	757	rBV	1273615	1734250	87.41%	6.285%
7	6.898	811	817	822	rBV	473812	597310	30.11%	2.165%
8	7.051	838	843	847	rVB	39726	47267	2.38%	0.171%
9	7.457	905	912	917	rBV	845122	1106456	55.77%	4.010%
10	7.857	972	980	987	rBV	20881	36647	1.85%	0.133%
11	8.175	1029	1034	1041	rBV	595213	787071	39.67%	2.852%
12	8.487	1083	1087	1092	rBV	47328	61464	3.10%	0.223%
13	9.128	1192	1196	1207	rVV2	26229	38833	1.96%	0.141%
14	9.251	1211	1217	1222	rVV	1552698	1984067	100.00%	7.190%
15	9.316	1222	1228	1232	rVV3	19127	29263	1.47%	0.106%
16	9.375	1232	1238	1248	rVB2	47762	74780	3.77%	0.271%
17	9.563	1266	1270	1272	rBV2	23236	31460	1.59%	0.114%
18	9.592	1272	1275	1278	rVV	65058	79319	4.00%	0.287%
19	9.633	1278	1282	1292	rVB	69484	87570	4.41%	0.317%
20	9.786	1303	1308	1315	rVB2	134345	184107	9.28%	0.667%
21	9.845	1315	1318	1324	rVV	44687	61023	3.08%	0.221%
22	9.910	1324	1329	1330	rVV	421778	501614	25.28%	1.818%
23	9.933	1330	1333	1345	rVV	719217	1013260	51.07%	3.672%
24	10.028	1345	1349	1351	rVV	40151	60105	3.03%	0.218%
25	10.057	1351	1354	1357	rVV	82760	104051	5.24%	0.377%
26	10.092	1357	1360	1364	rVV2	68142	85709	4.32%	0.311%
27	10.139	1364	1368	1375	rVB3	17520	30735	1.55%	0.111%
28	10.633	1447	1452	1455	rBV3	32564	44777	2.26%	0.162%
29	10.716	1455	1466	1471	rVV	1033973	1395283	70.32%	5.056%
30	10.757	1471	1473	1477	rVB3	23478	27281	1.38%	0.099%
31	10.839	1483	1487	1492	rVB	24431	33021	1.66%	0.120%
32	10.916	1496	1500	1505	rVV3	24238	47302	2.38%	0.171%
33	10.963	1506	1508	1513	rVB2	16737	20161	1.02%	0.073%
34	11.216	1547	1551	1556	rVB2	19651	27508	1.39%	0.100%
35	11.416	1580	1585	1593	rBV2	671775	1143248	57.62%	4.143%
36	11.492	1593	1598	1601	rVB	33918	46112	2.32%	0.167%

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Integrator: RTE

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Start Thrs: 0.2

Max Peaks: 100

Stop Thrs : 0

Peak Location: TOP

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

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 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	11.645	1619	1624	1631	rBV	22497	33556	1.69%	0.122%
38	11.722	1631	1637	1646	rVB8	22878	51077	2.57%	0.185%
39	11.916	1665	1670	1671	rBV2	34574	46703	2.35%	0.169%
40	11.945	1671	1675	1681	rVB	221179	295114	14.87%	1.069%
41	12.027	1686	1689	1697	rVV2	45776	89779	4.52%	0.325%
42	12.116	1699	1704	1713	rVV5	20088	45897	2.31%	0.166%
43	12.233	1717	1724	1729	rVB2	49275	86693	4.37%	0.314%
44	12.551	1774	1778	1785	rVB	38526	52800	2.66%	0.191%
45	12.627	1786	1791	1795	rBV	461356	644034	32.46%	2.334%
46	12.733	1805	1809	1815	rBV3	49915	71921	3.62%	0.261%
47	12.857	1823	1830	1835	rBV	338244	500324	25.22%	1.813%
48	12.904	1836	1838	1843	rVB2	20740	24709	1.25%	0.090%
49	13.004	1847	1855	1860	rVB	1315001	1657427	83.54%	6.006%
50	13.074	1860	1867	1870	rBV4	23334	39427	1.99%	0.143%
51	13.110	1870	1873	1878	rVB2	31351	46681	2.35%	0.169%
52	13.186	1878	1886	1888	rBV2	36338	68694	3.46%	0.249%
53	13.216	1888	1891	1894	rVV	44634	58099	2.93%	0.211%
54	13.251	1894	1897	1900	rVV2	26788	35328	1.78%	0.128%
55	13.410	1921	1924	1928	rVB	20786	23170	1.17%	0.084%
56	13.580	1946	1953	1957	rBV8	16863	36657	1.85%	0.133%
57	13.663	1963	1967	1969	rBV2	21059	26871	1.35%	0.097%
58	13.692	1969	1972	1977	rVB2	29095	41897	2.11%	0.152%
59	13.774	1980	1986	1994	rBV	1243270	1635704	82.44%	5.928%
60	13.910	2003	2009	2025	rBV3	145291	294890	14.86%	1.069%
61	14.057	2025	2034	2043	rBV2	503042	977043	49.24%	3.541%
62	14.157	2047	2051	2055	rVB2	23282	34169	1.72%	0.124%
63	14.233	2061	2064	2068	rBV3	14566	22699	1.14%	0.082%
64	14.351	2080	2084	2091	rVB2	39537	54524	2.75%	0.198%
65	14.439	2095	2099	2102	rVV	22694	32274	1.63%	0.117%
66	14.474	2102	2105	2109	rVB2	29263	37232	1.88%	0.135%
67	14.539	2111	2116	2132	rBV2	229061	508670	25.64%	1.843%
68	14.751	2147	2152	2162	rBV6	30697	62020	3.13%	0.225%
69	14.845	2162	2168	2171	rBV3	21849	44970	2.27%	0.163%
70	14.921	2177	2181	2187	rVB4	14417	25636	1.29%	0.093%
71	14.998	2189	2194	2202	rVB2	121754	175415	8.84%	0.636%
72	15.098	2205	2211	2222	rBV	202732	458546	23.11%	1.662%
73	15.198	2222	2228	2231	rBV	230662	369945	18.65%	1.341%
74	15.368	2253	2257	2259	rBV2	22861	33652	1.70%	0.122%
75	15.404	2259	2263	2268	rVB	102445	154178	7.77%	0.559%
76	15.468	2268	2274	2279	rBV	115053	176409	8.89%	0.639%

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77	15.533	2279	2285	2298	rVB	335820	585119	29.49%	2.120%
78	15.792	2324	2329	2337	rVB	169337	282732	14.25%	1.025%
79	16.039	2364	2371	2376	rBV	199960	361570	18.22%	1.310%
80	16.092	2376	2380	2387	rVV	86258	212708	10.72%	0.771%
81	16.157	2388	2391	2400	rVB	52261	109470	5.52%	0.397%
82	16.286	2408	2413	2422	rVB5	19922	48134	2.43%	0.174%
83	16.562	2455	2460	2466	rBV5	12392	24401	1.23%	0.088%
84	16.857	2501	2510	2519	rVB3	120898	273249	13.77%	0.990%
85	17.009	2530	2536	2541	rBV2	63988	133574	6.73%	0.484%
86	17.080	2542	2548	2558	rVB9	34810	120784	6.09%	0.438%
87	17.174	2558	2564	2571	rBV2	43709	103925	5.24%	0.377%
88	17.262	2572	2579	2590	rVV5	56112	217057	10.94%	0.787%
89	17.362	2591	2596	2605	rVV2	49625	128508	6.48%	0.466%
90	17.451	2605	2611	2619	rVB	47524	98409	4.96%	0.357%
91	17.645	2636	2644	2671	rBV4	115286	446546	22.51%	1.618%
92	17.998	2696	2704	2710	rBV10	20896	68763	3.47%	0.249%
93	18.339	2756	2762	2777	rVB7	22119	73917	3.73%	0.268%
94	18.692	2816	2822	2829	rVB7	11946	34228	1.73%	0.124%

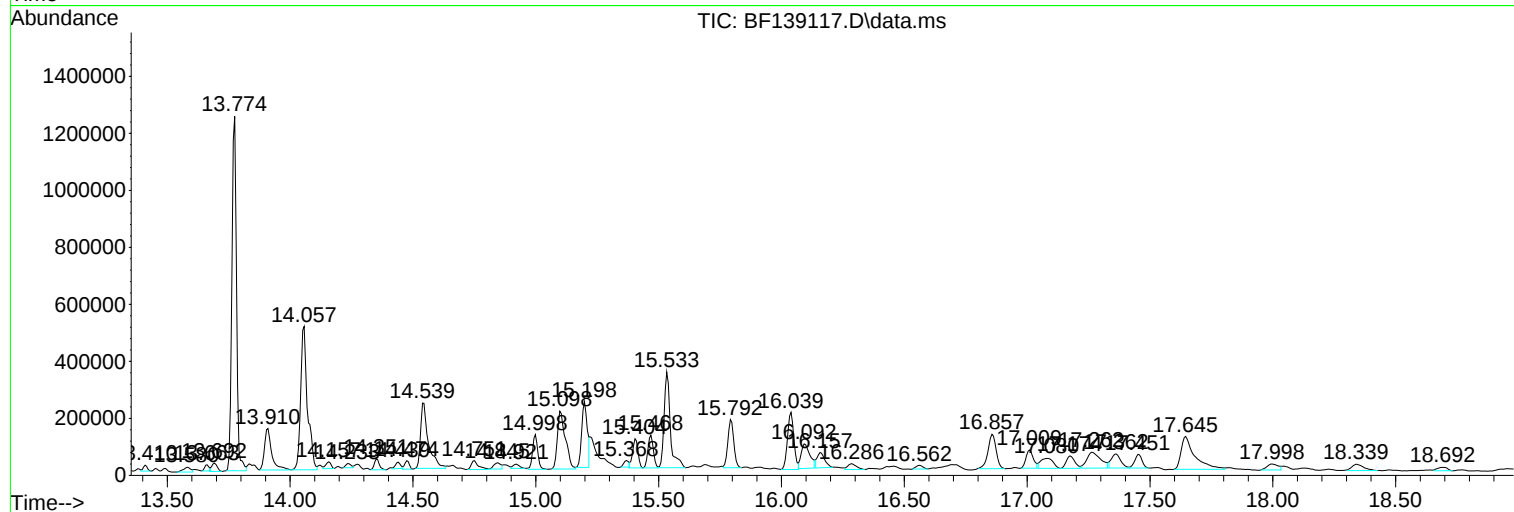
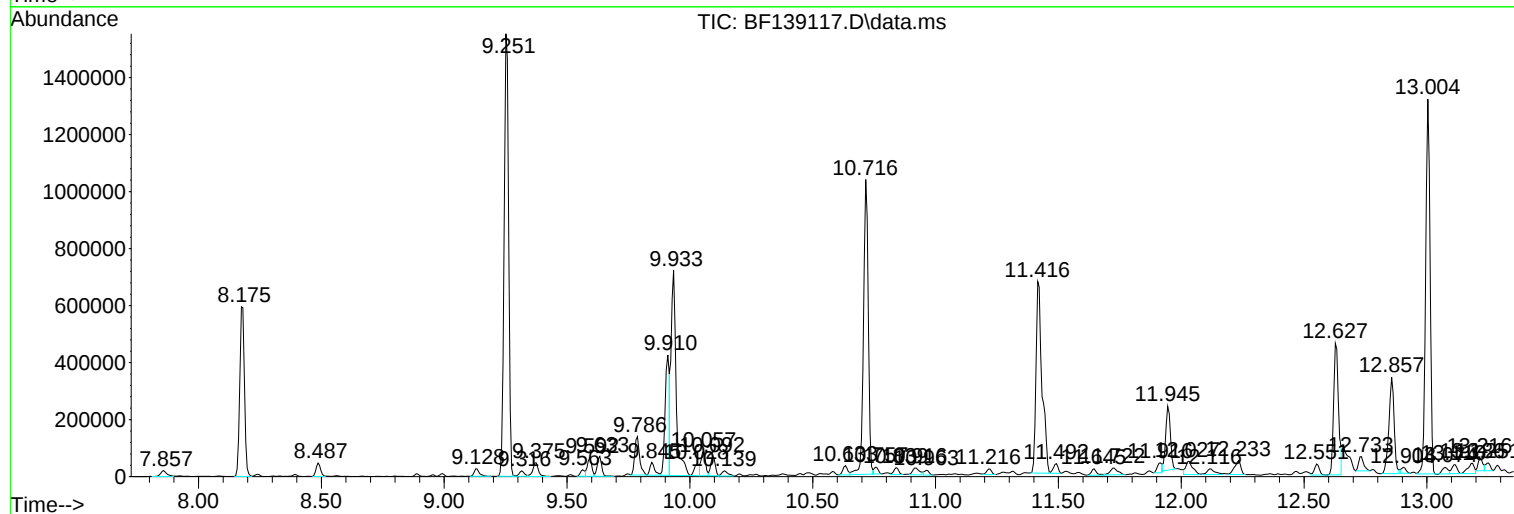
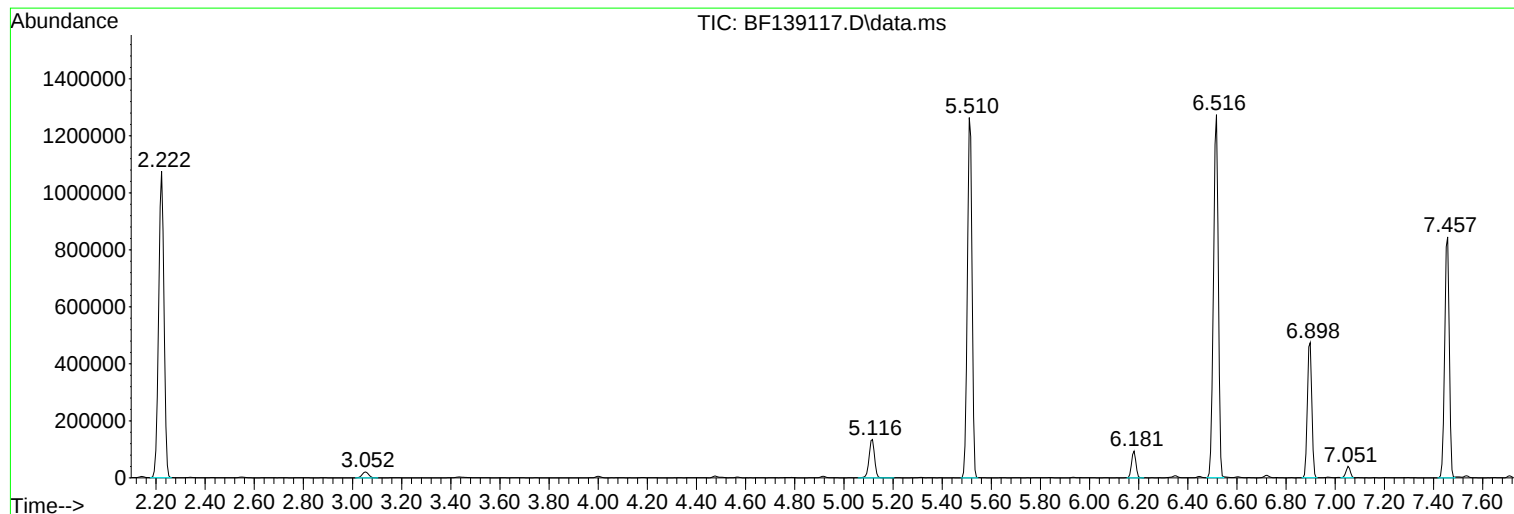
Sum of corrected areas: 27594533

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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF082024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082224\
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Sample : P3641-04
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
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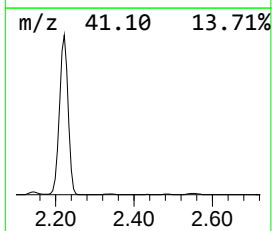
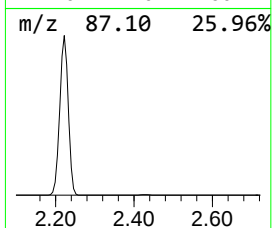
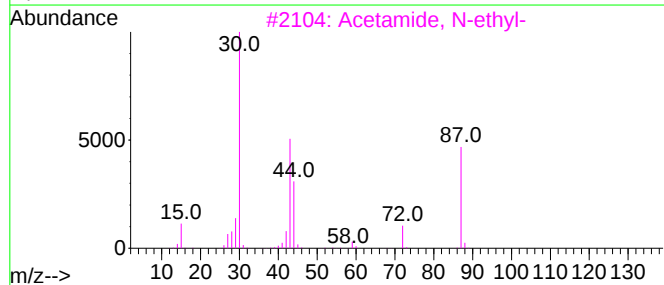
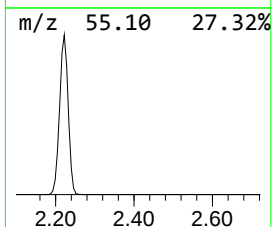
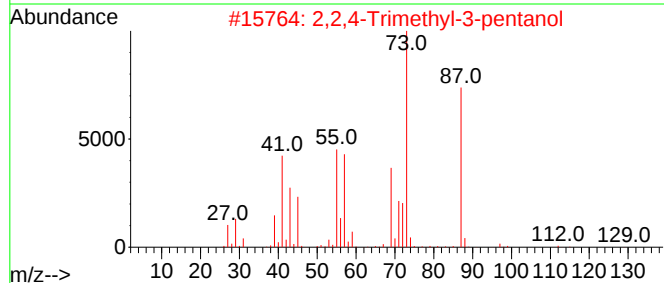
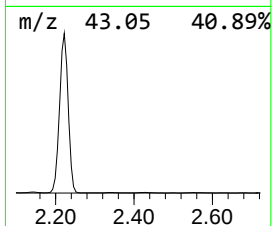
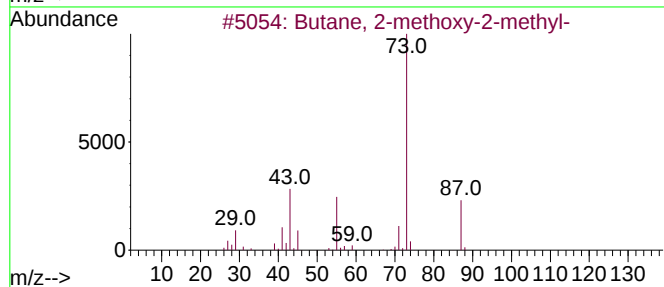
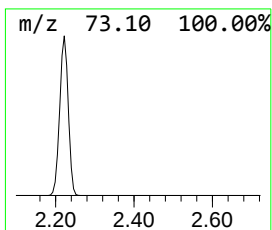
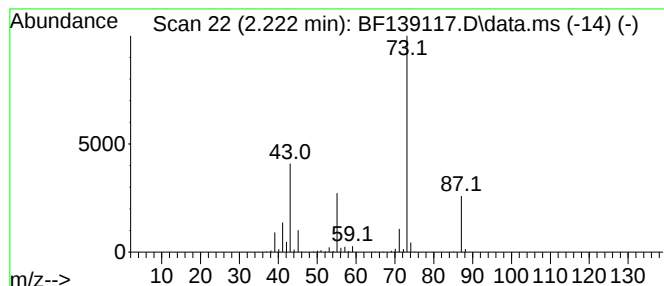
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF082024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.222	54.56 ng	1629570	1,4-Dichlorobenzene-d4	6.898

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3			Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	27
4			Octanal, 7-methoxy-3,7-dimethyl-	186	C11H22O2	003613-30-7	17
5			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12



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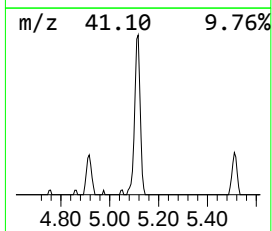
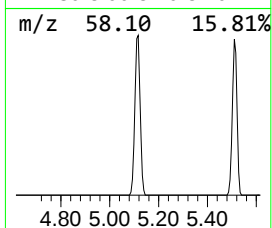
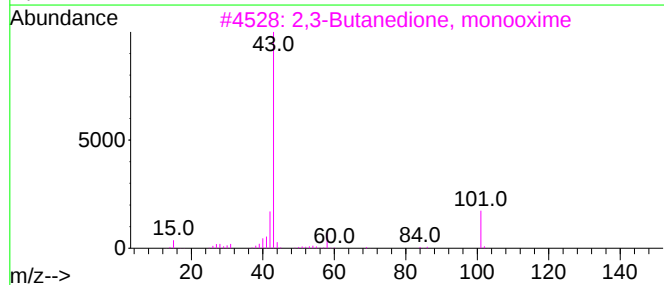
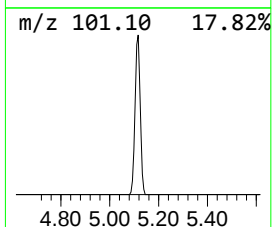
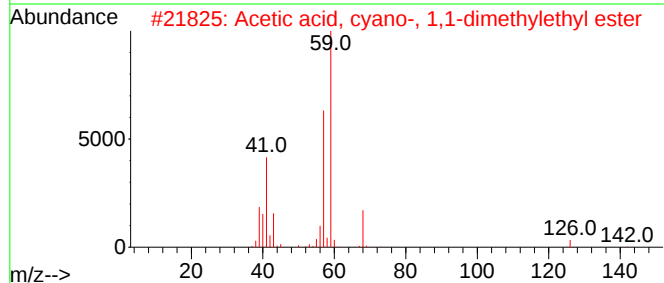
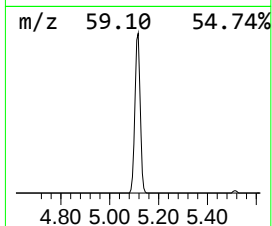
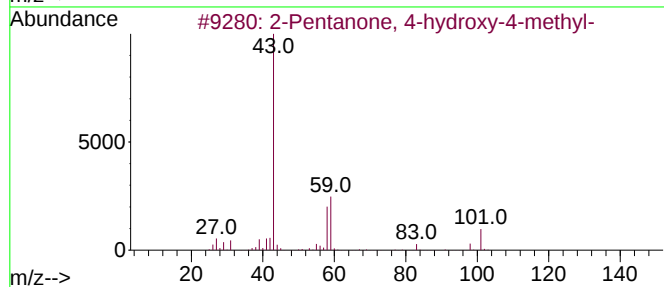
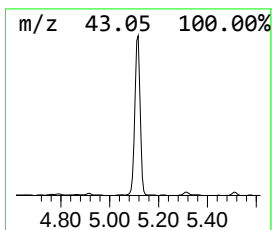
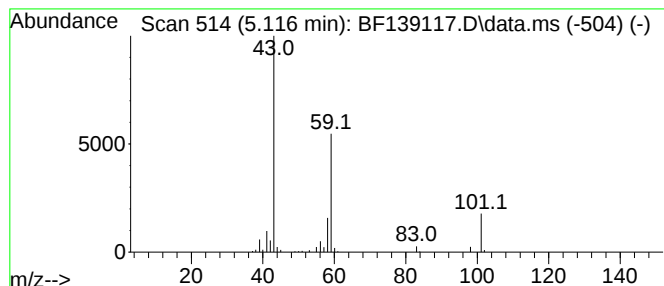
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.116	7.04 ng	210255	1,4-Dichlorobenzene-d4	6.898

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	32
3			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16
4			Acetone	58	C3H6O	000067-64-1	12
5			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12



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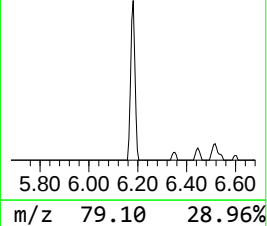
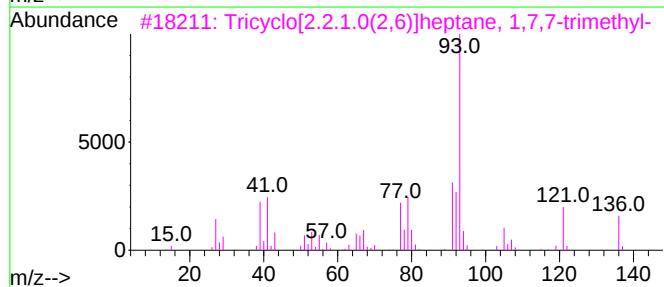
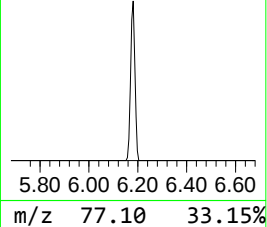
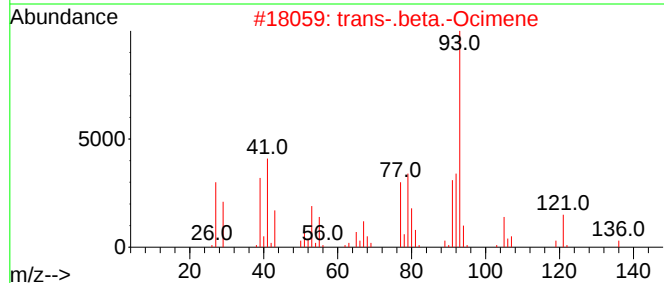
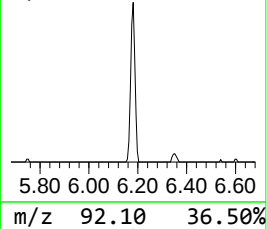
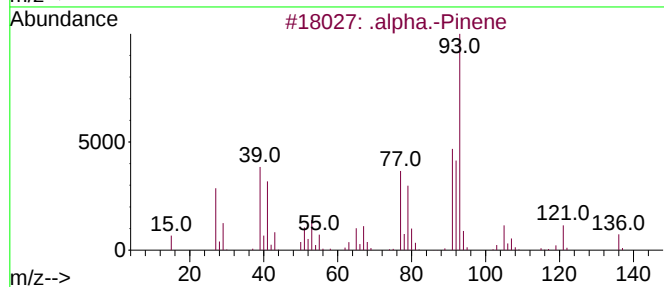
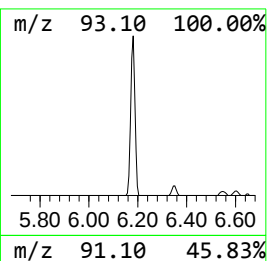
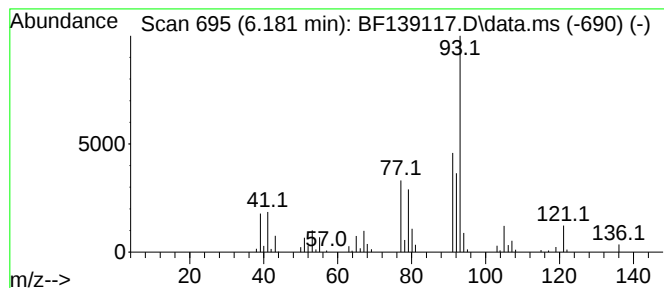
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF082024.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 .alpha.-Pinene Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.181	3.86 ng	115236	1,4-Dichlorobenzene-d4	6.898

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		.alpha.-Pinene	136	C10H16	000080-56-8	94
2		trans-.beta.-Ocimene	136	C10H16	003779-61-1	94
3		Tricyclo[2.2.1.0(2,6)]heptane, 1...	136	C10H16	000508-32-7	91
4		3-Carene	136	C10H16	013466-78-9	91
5		Bicyclo[3.1.1]hept-2-ene, 3,6,6-...	136	C10H16	004889-83-2	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082224\
Data File : BF139117.D
Acq On : 22 Aug 2024 12:22
Operator : RC/JU
Sample : P3641-04
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
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S-908-K1-0.5-1.0-081524

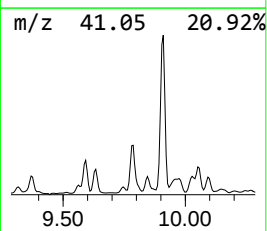
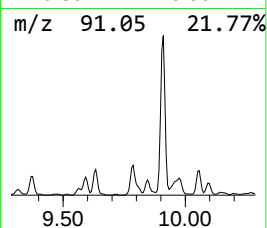
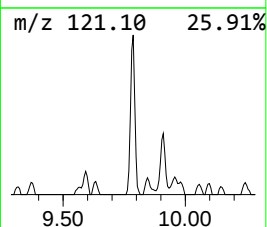
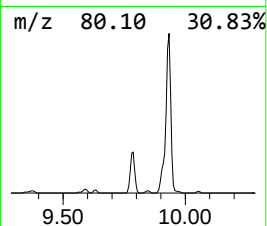
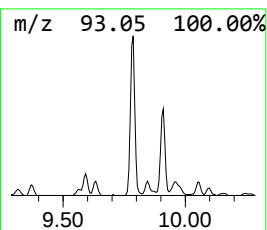
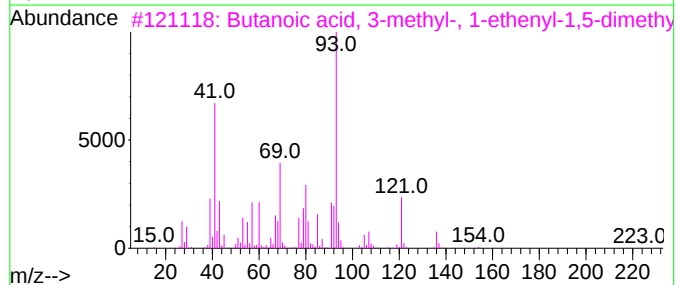
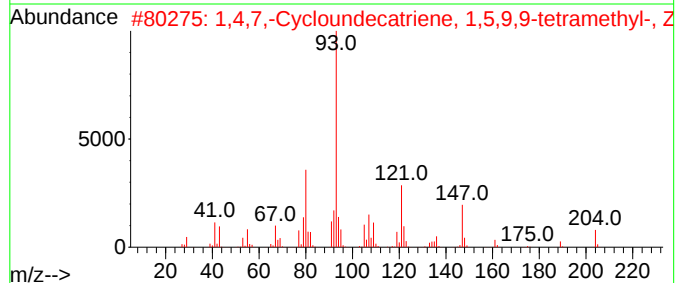
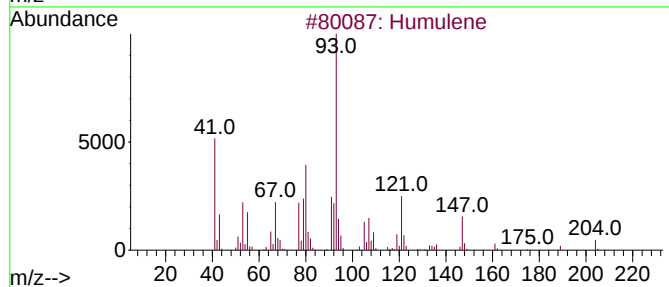
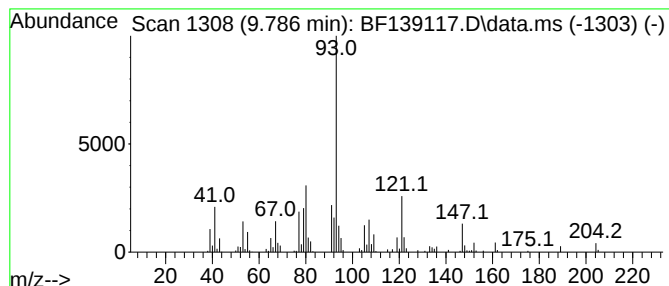
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 Humulene Concentration Rank 20

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.786	3.63 ng	184107	Acenaphthene-d10	9.933

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Humulene	204	C15H24	006753-98-6	97
2			1,4,7,-Cycloundecatriene, 1,5,9,...	204	C15H24	1000062-61-9	90
3			Butanoic acid, 3-methyl-, 1-ethe...	238	C15H26O2	001118-27-0	64
4			Tricyclo[2.2.1.0(2,6)]heptane, 1...	136	C10H16	000488-97-1	59
5			Bicyclo[3.1.0]hexan-2-ol, 2-meth...	154	C10H18O	017699-16-0	50



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082224\
Data File : BF139117.D
Acq On : 22 Aug 2024 12:22
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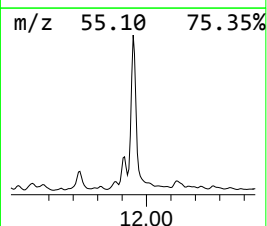
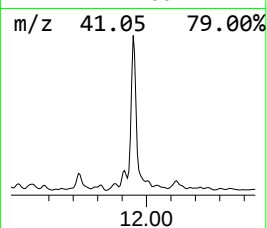
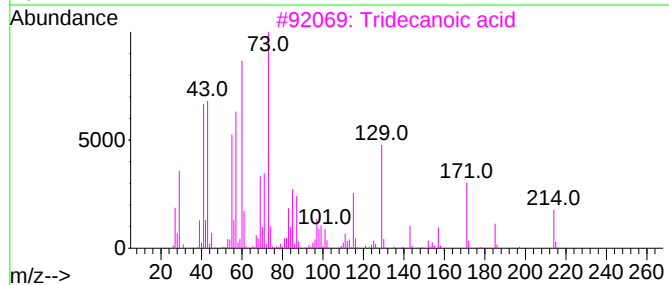
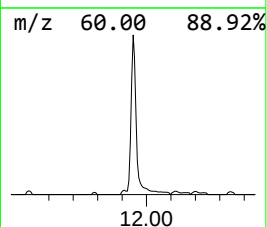
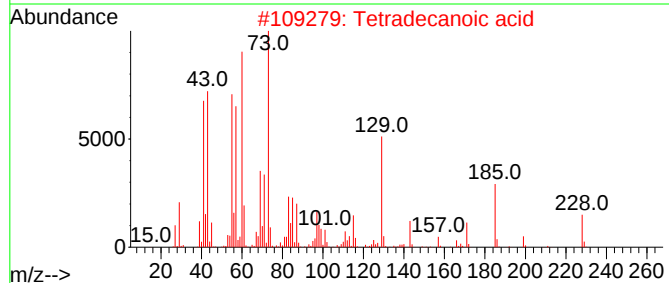
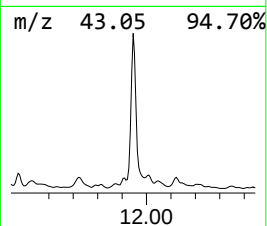
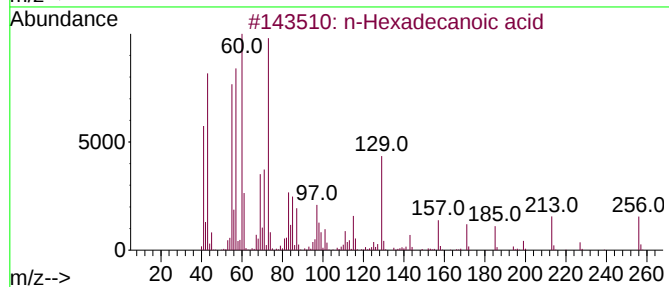
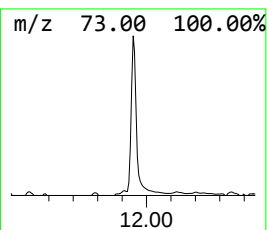
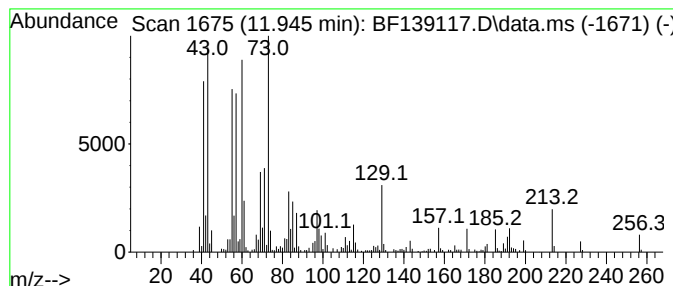
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 n-Hexadecanoic acid Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.945	5.16 ng	295114	Phenanthrene-d10	11.416

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Tetradecanoic acid	228	C14H28O2	000544-63-8	91
3			Tridecanoic acid	214	C13H26O2	000638-53-9	83
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	81
5			Octanoic acid	144	C8H16O2	000124-07-2	45



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082224\
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Misc :
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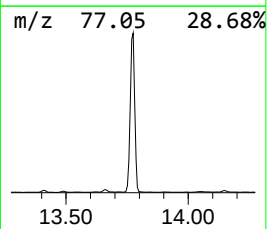
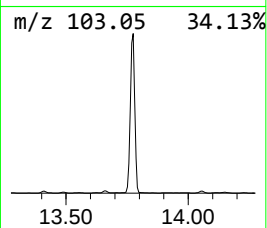
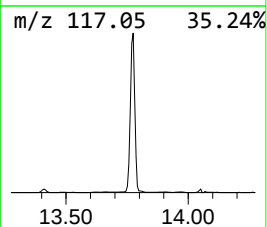
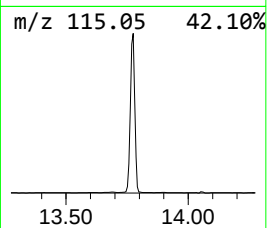
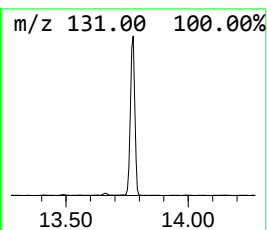
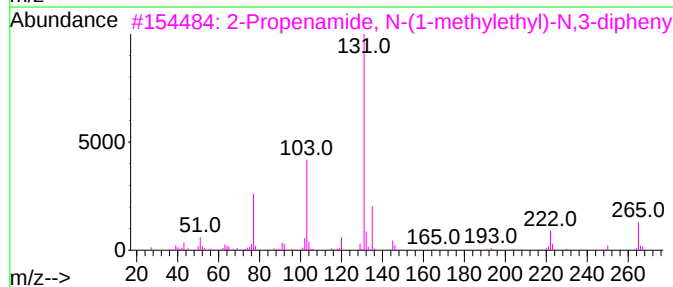
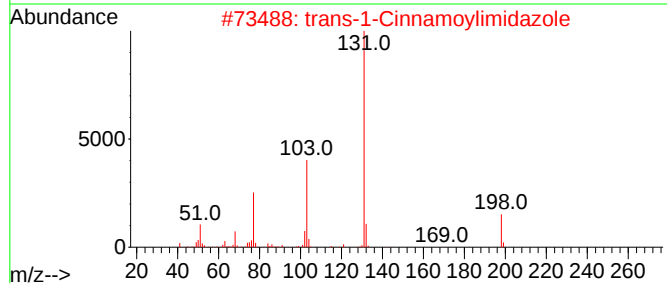
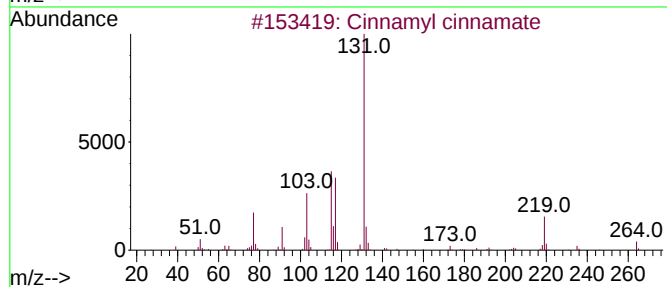
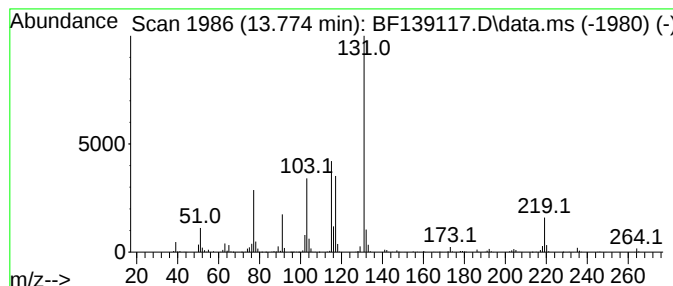
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Cinnamyl cinnamate Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.774	33.48 ng	1635700	Chrysene-d12	14.057

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cinnamyl cinnamate	264	C18H16O2	000122-69-0	91
2			trans-1-Cinnamoylimidazole	198	C12H10N2O	001138-15-4	47
3			2-Propenamide, N-(1-methylethyl)...	265	C18H19NO	055044-37-6	47
4			1-Penten-3-one, 4,4-dimethyl-1-p...	188	C13H16O	000538-44-3	47
5			2,2-Dimethyl-1-(2-vinylphenyl)pr...	188	C13H16O	1000210-99-9	47



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082224\
Data File : BF139117.D
Acq On : 22 Aug 2024 12:22
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Sample : P3641-04
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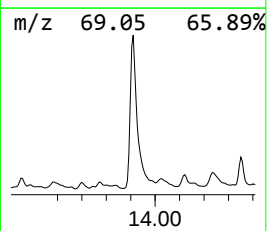
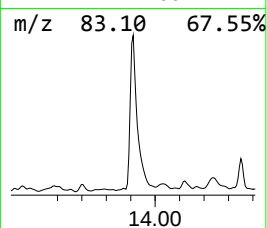
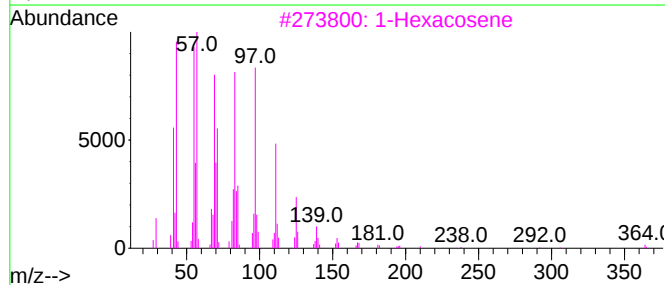
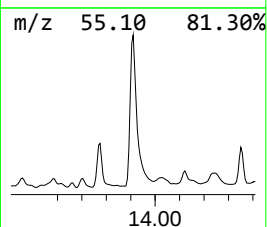
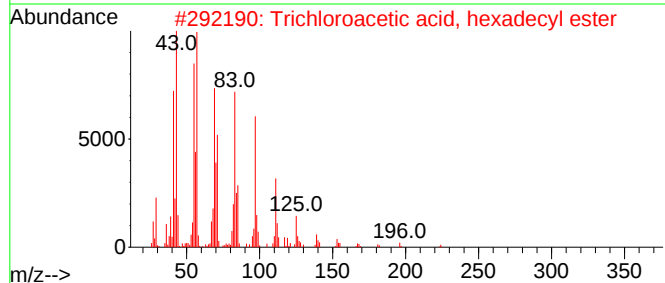
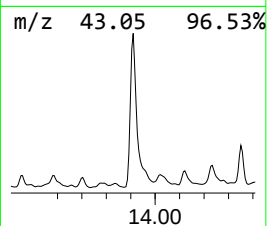
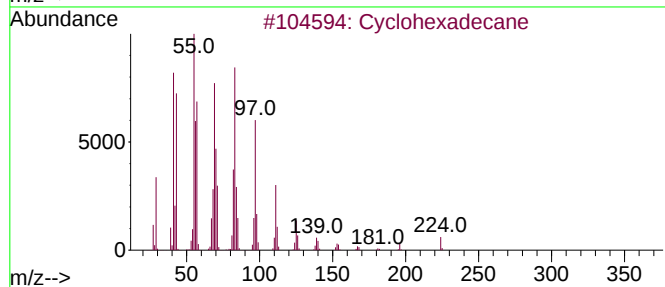
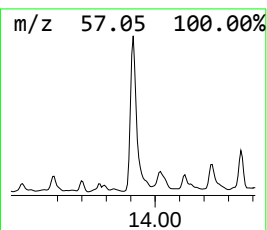
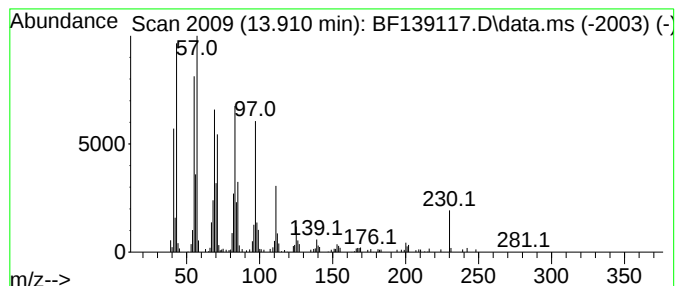
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Cyclohexadecane Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.910	6.04 ng	294890	Chrysene-d12	14.057

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexadecane	224	C16H32	000295-65-8	98
2			Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	93
3			1-Hexacosene	364	C26H52	018835-33-1	91
4			Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	91
5			Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082224\
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Operator : RC/JU
Sample : P3641-04
Misc :
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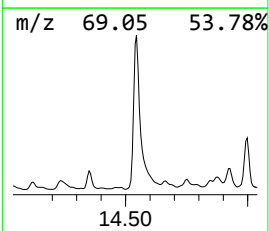
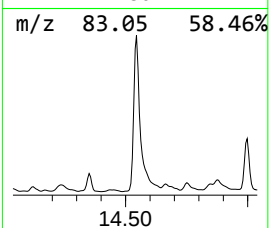
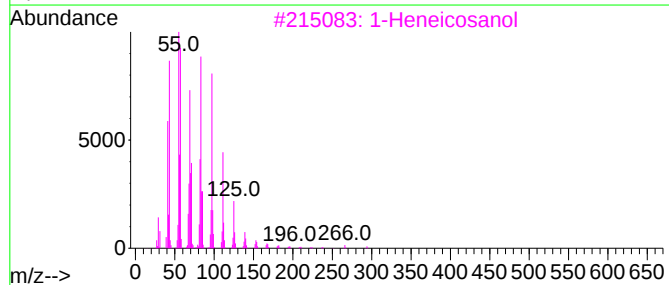
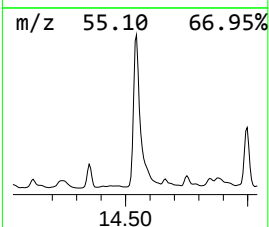
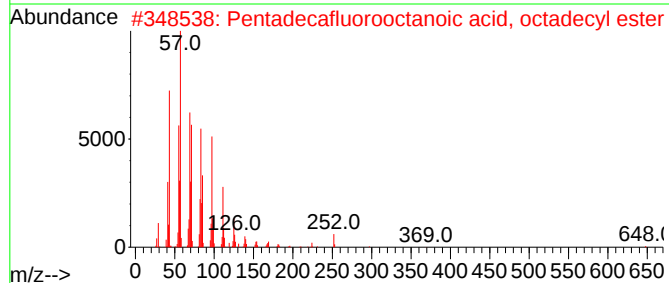
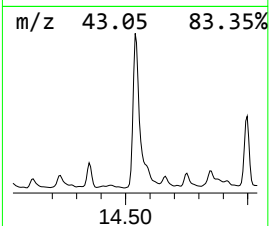
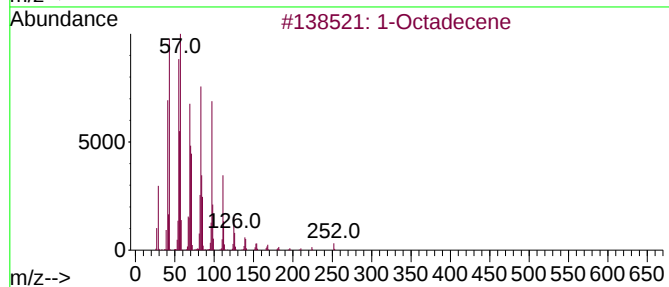
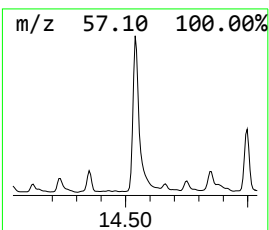
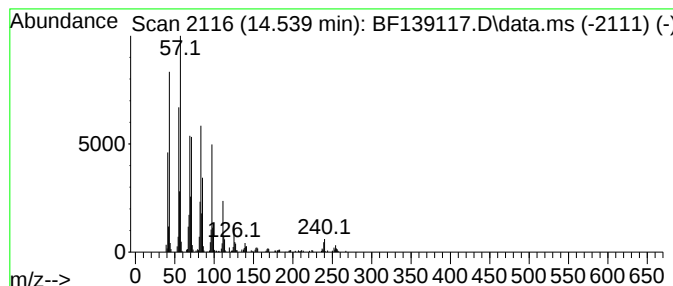
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 8 1-Octadecene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.539	10.41 ng	508670	Chrysene-d12	14.057

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Octadecene	252	C18H36	000112-88-9	97
2			Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	94
3			1-Heneicosanol	312	C21H44O	015594-90-8	93
4			1-Hexacosene	364	C26H52	018835-33-1	93
5			Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082224\
Data File : BF139117.D
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Sample : P3641-04
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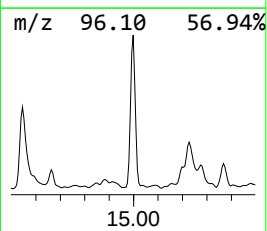
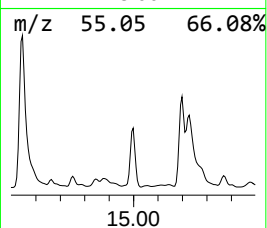
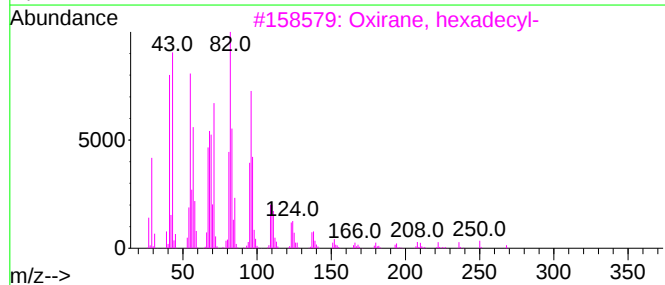
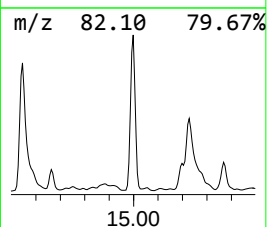
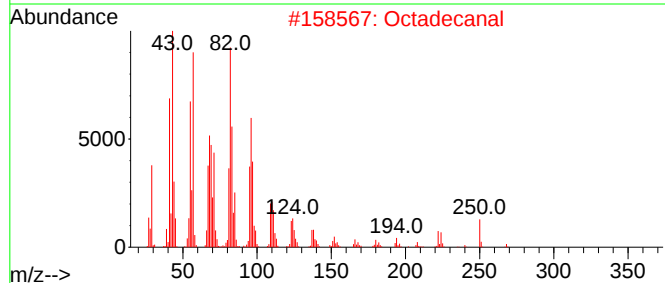
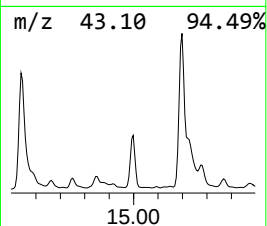
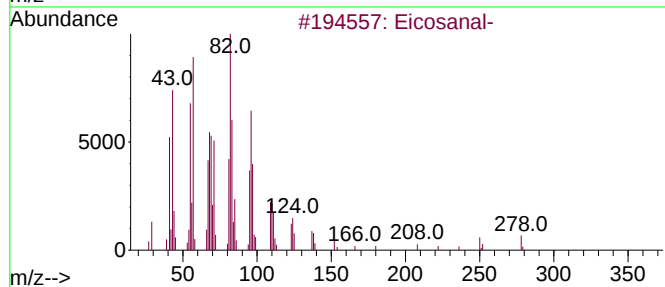
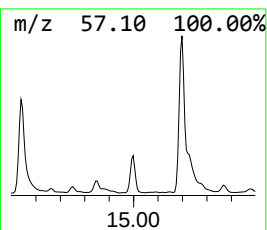
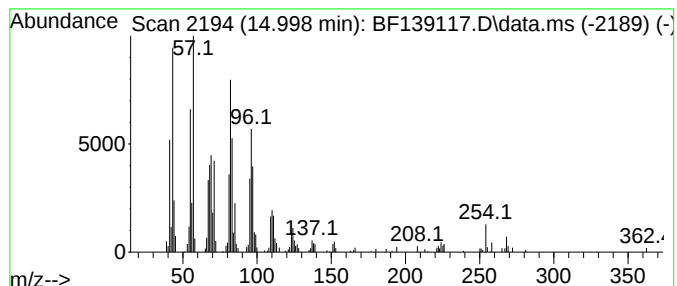
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Eicosanal- Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.998	6.00 ng	175415	Perylene-d12	15.533

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Eicosanal-	296	C20H40O	002400-66-0	94
2			Octadecanal	268	C18H36O	000638-66-4	91
3			Oxirane, hexadecyl-	268	C18H36O	007390-81-0	91
4			Hexacosanal	380	C26H52O	026627-85-0	91
5			Hexadecanal	240	C16H32O	000629-80-1	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082224\
Data File : BF139117.D
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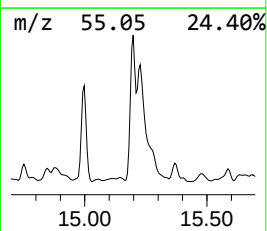
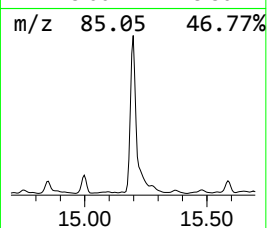
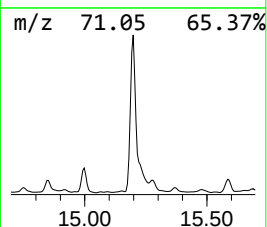
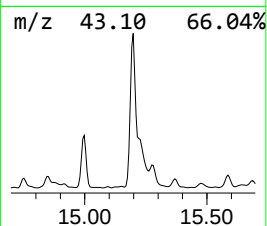
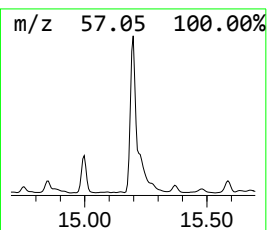
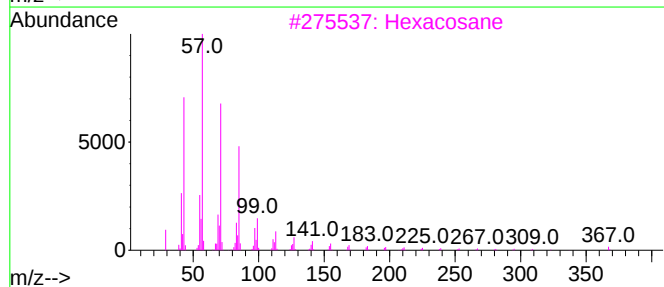
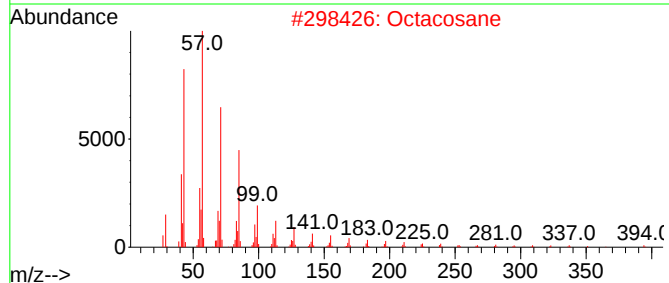
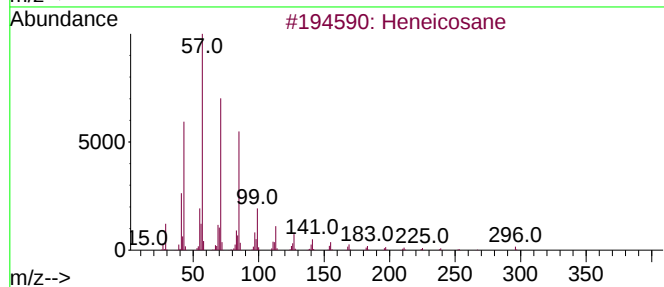
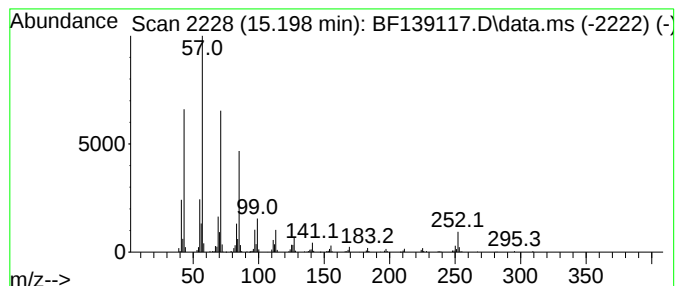
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Heneicosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.198	12.65 ng	369945	Perylene-d12	15.533

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Heneicosane	296	C21H44	000629-94-7	87
2		Octacosane	394	C28H58	000630-02-4	87
3		Hexacosane	366	C26H54	000630-01-3	87
4		Tetracosane	338	C24H50	000646-31-1	87
5		Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082224\
Data File : BF139117.D
Acq On : 22 Aug 2024 12:22
Operator : RC/JU
Sample : P3641-04
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
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ClientSampleId :
S-908-K1-0.5-1.0-081524

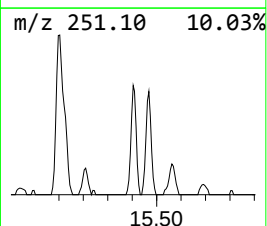
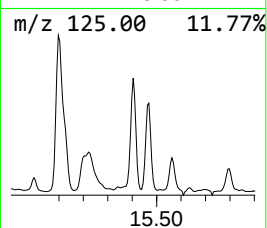
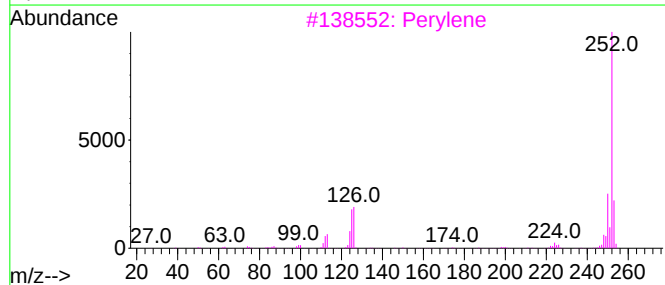
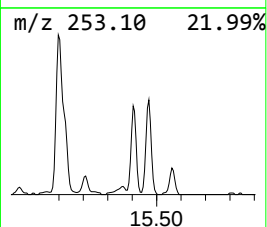
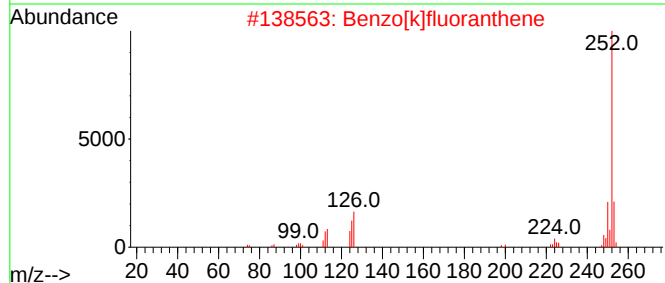
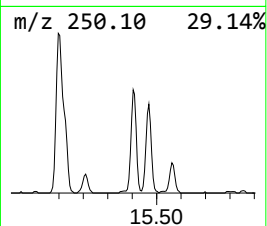
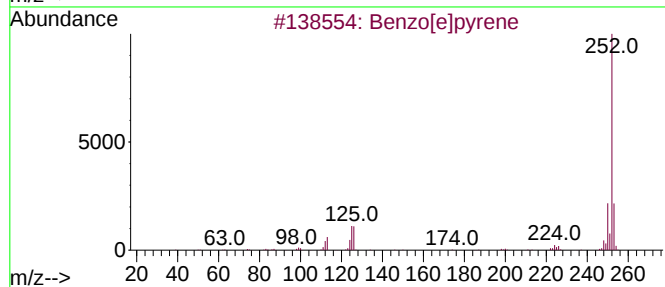
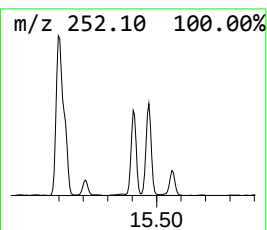
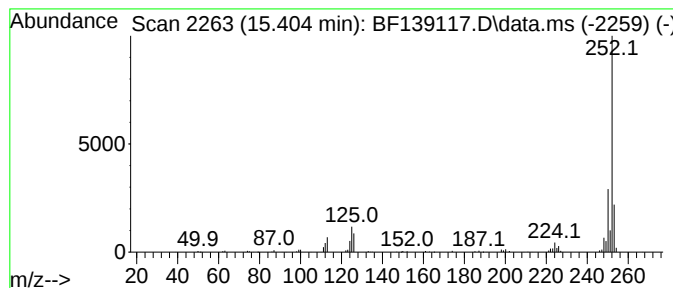
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Benzo[e]pyrene Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.404	5.27 ng	154178	Perylene-d12	15.533

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzo[e]pyrene	252	C20H12	000192-97-2	97
2			Benzo[k]fluoranthene	252	C20H12	000207-08-9	96
3			Perylene	252	C20H12	000198-55-0	94
4			Benzo[b]fluoranthene	252	C20H12	000205-99-2	93
5			Benzo[j]fluoranthene	252	C20H12	000205-82-3	93



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082224\
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Operator : RC/JU
Sample : P3641-04
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ClientSampleId :
S-908-K1-0.5-1.0-081524

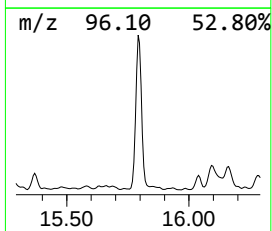
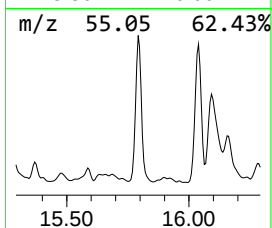
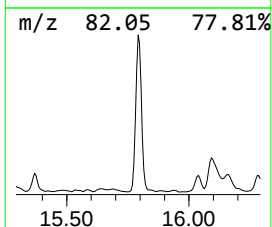
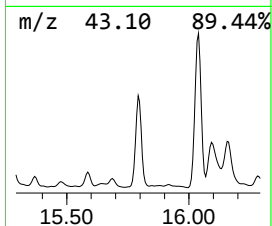
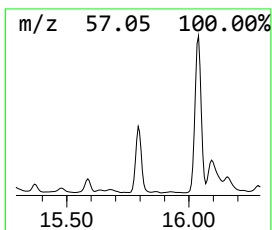
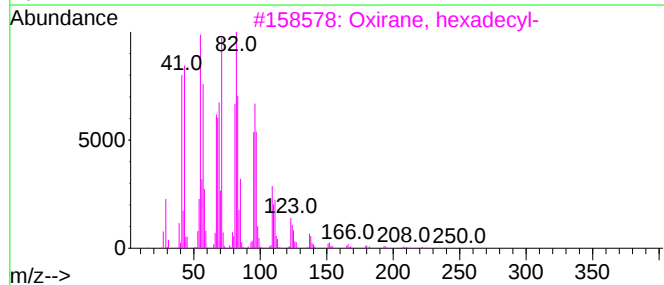
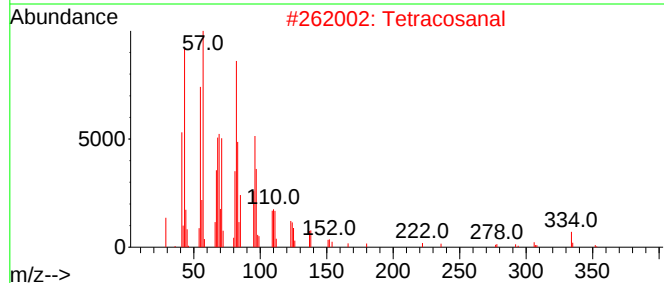
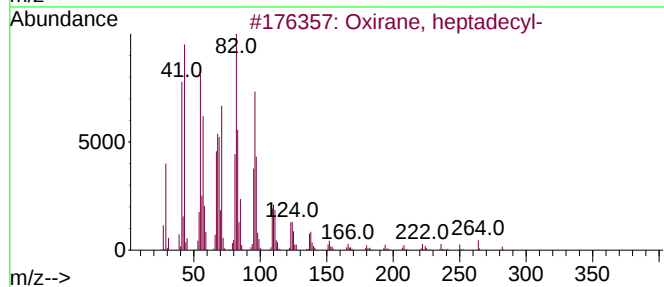
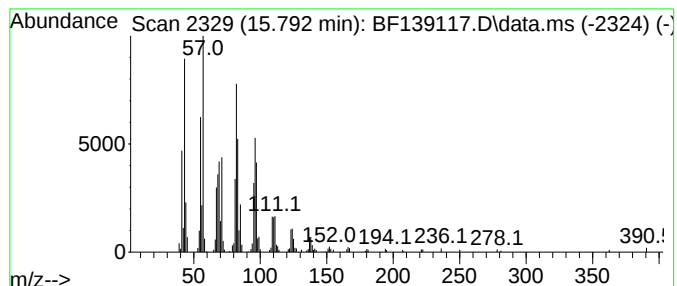
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Oxirane, heptadecyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.792	9.66 ng	282732	Perylene-d12	15.533

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Oxirane, heptadecyl-	282	C19H38O	067860-04-2	94
2			Tetracosanal	352	C24H48O	057866-08-7	94
3			Oxirane, hexadecyl-	268	C18H36O	007390-81-0	91
4			Octadecanal	268	C18H36O	000638-66-4	91
5			Octacosanal	408	C28H56O	022725-64-0	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082224\
Data File : BF139117.D
Acq On : 22 Aug 2024 12:22
Operator : RC/JU
Sample : P3641-04
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Instrument :
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ClientSampleId :
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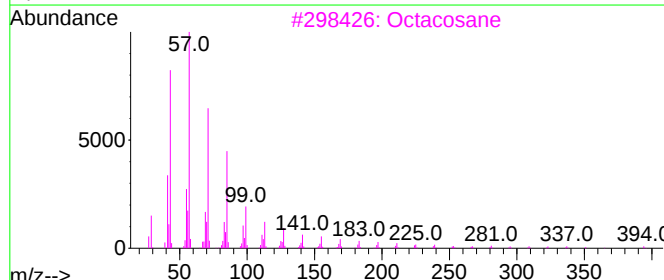
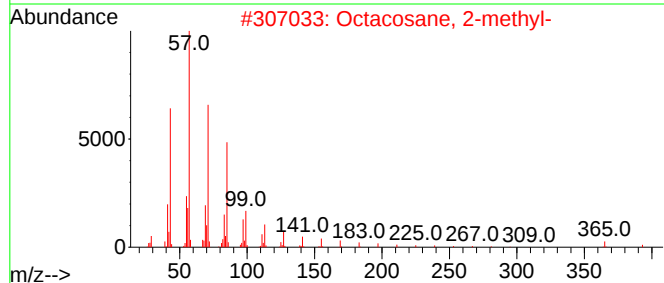
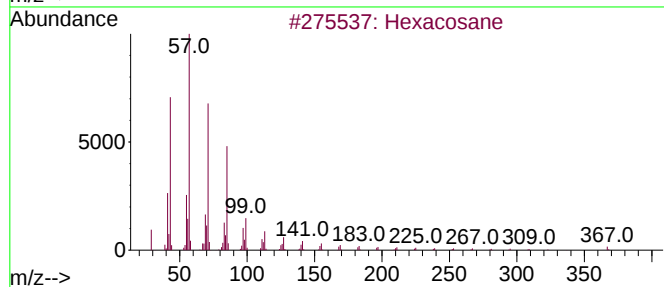
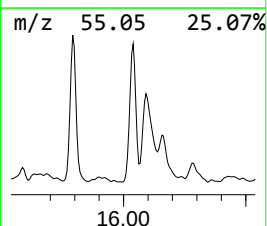
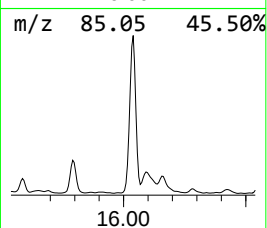
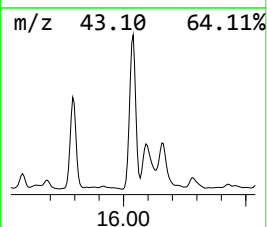
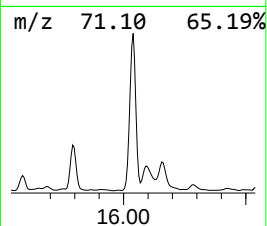
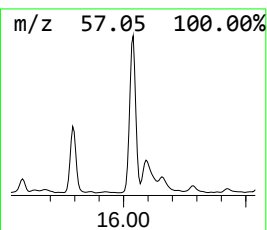
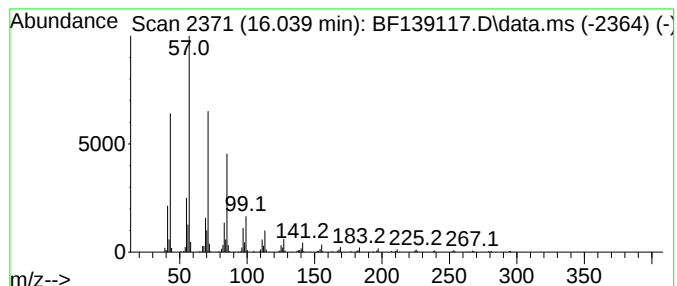
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 Hexacosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.039	12.36 ng	361570	Perylene-d12	15.533

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexacosane	366	C26H54	000630-01-3	94
2			Octacosane, 2-methyl-	408	C29H60	001560-98-1	91
3			Octacosane	394	C28H58	000630-02-4	91
4			Heneicosane	296	C21H44	000629-94-7	91
5			Triacontane	422	C30H62	000638-68-6	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082224\
Data File : BF139117.D
Acq On : 22 Aug 2024 12:22
Operator : RC/JU
Sample : P3641-04
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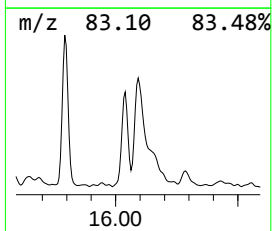
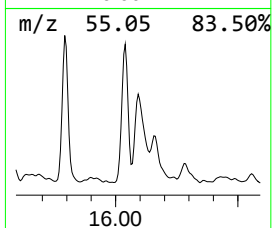
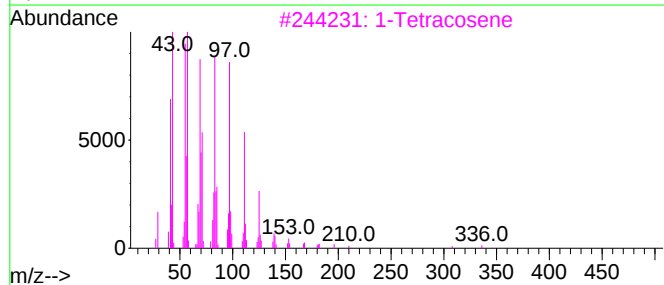
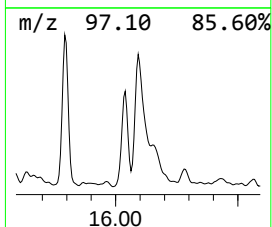
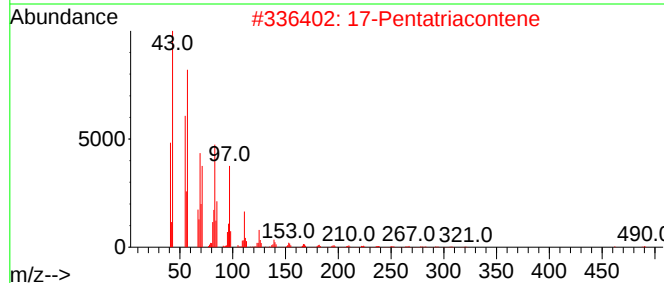
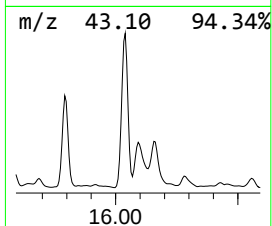
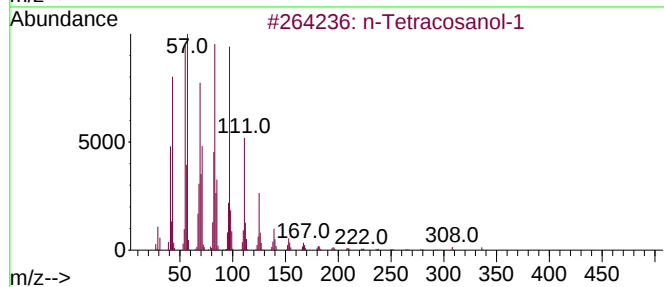
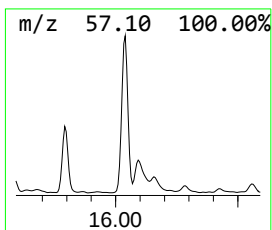
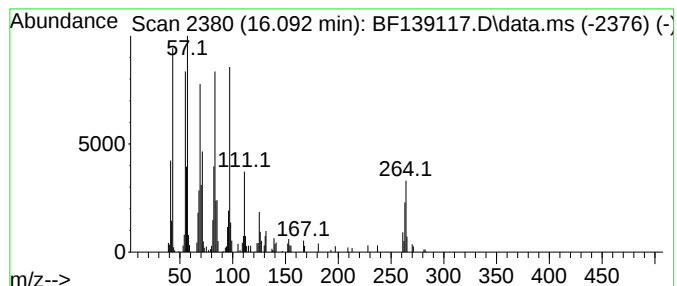
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 14 n-Tetracosanol-1 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.092	7.27 ng	212708	Perylene-d12	15.533

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Tetracosanol-1	354	C24H50O	000506-51-4	91
2			17-Pentatriacontene	491	C35H70	006971-40-0	74
3			1-Tetracosene	336	C24H48	010192-32-2	70
4			Octacosanol	410	C28H58O	000557-61-9	60
5			11-Tricosene	322	C23H46	052078-56-5	58



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082224\
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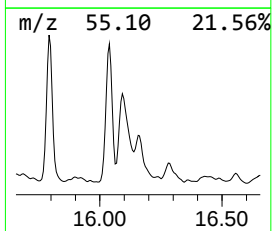
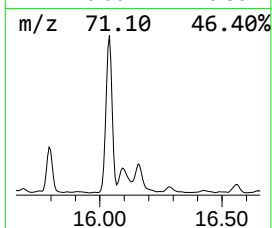
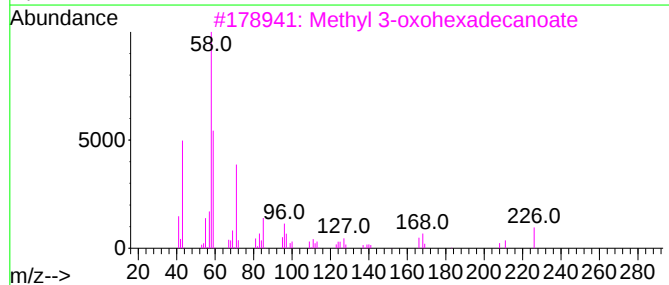
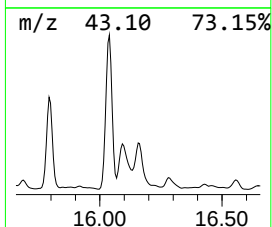
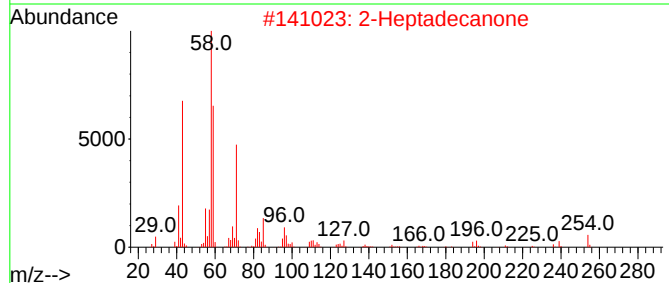
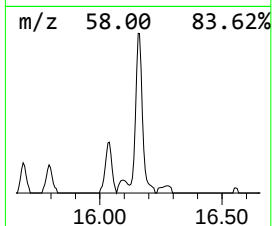
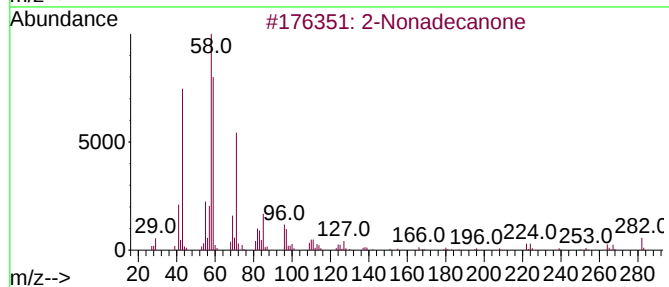
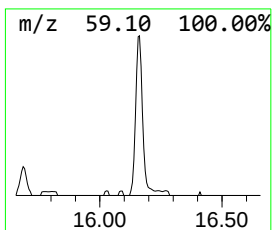
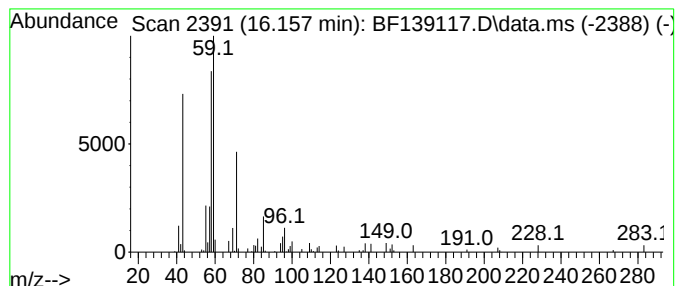
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 15 2-Nonadecanone Concentration Rank 19

R.T.	EstConc	Area	Relative to ISTD	R.T.	
16.157	3.74 ng	109470	Perylene-d12	15.533	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Nonadecanone	282	C19H38O	000629-66-3	59
2	2-Heptadecanone	254	C17H34O	002922-51-2	59
3	Methyl 3-oxohexadecanoate	284	C17H32O3	1010429-04-8	59
4	Oxirane, tetramethyl-	100	C6H12O	005076-20-0	52
5	2-Pentadecanone	226	C15H30O	002345-28-0	45



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082224\
Data File : BF139117.D
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Sample : P3641-04
Misc :
ALS Vial : 6 Sample Multiplier: 1

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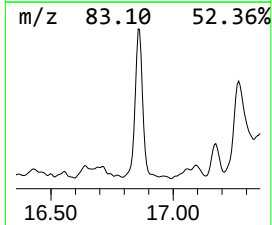
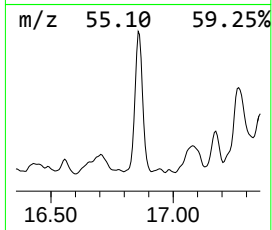
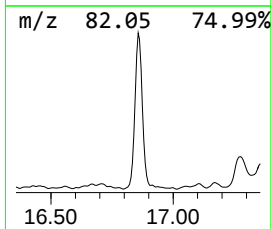
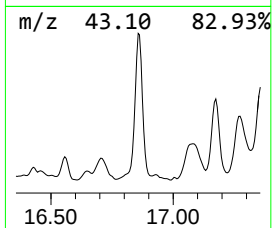
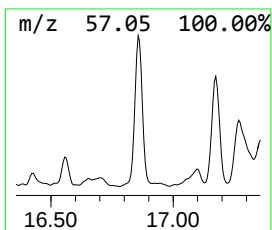
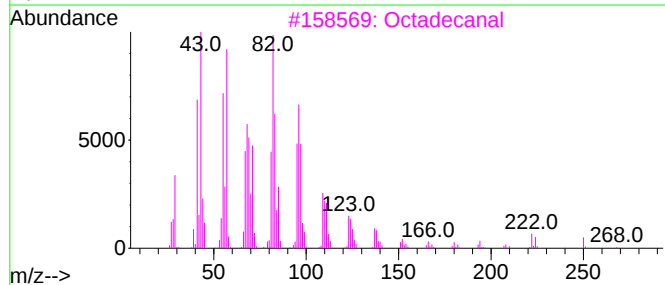
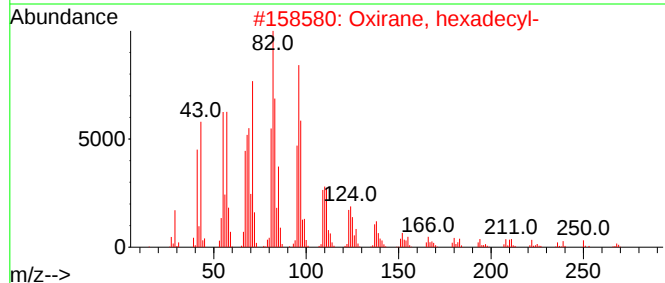
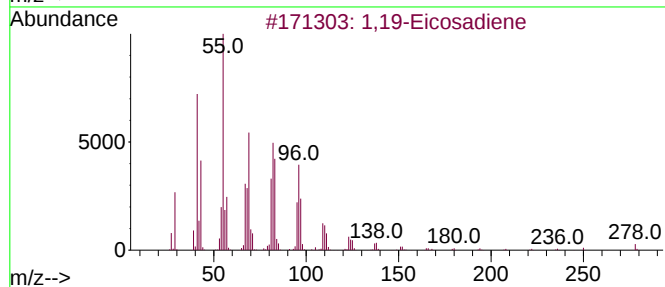
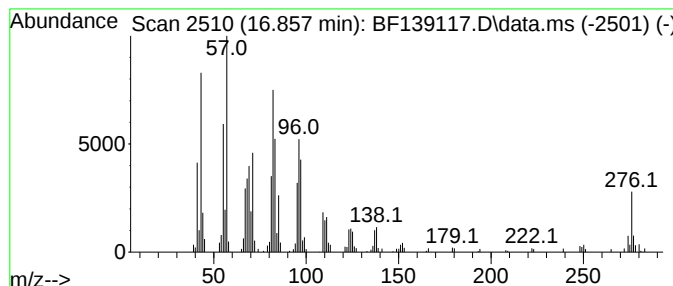
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 16 1,19-Eicosadiene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.857	9.34 ng	273249	Perylene-d12	15.533

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,19-Eicosadiene	278	C20H38	014811-95-1	91
2			Oxirane, hexadecyl-	268	C18H36O	007390-81-0	90
3			Octadecanal	268	C18H36O	000638-66-4	87
4			Oxirane, heptadecyl-	282	C19H38O	067860-04-2	81
5			1-Eicosyne	278	C20H38	000765-27-5	70



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082224\
Data File : BF139117.D
Acq On : 22 Aug 2024 12:22
Operator : RC/JU
Sample : P3641-04
Misc :
ALS Vial : 6 Sample Multiplier: 1

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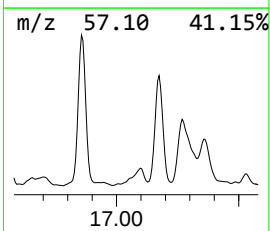
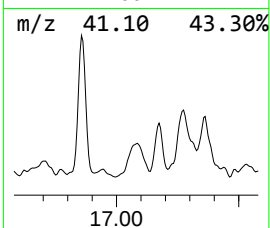
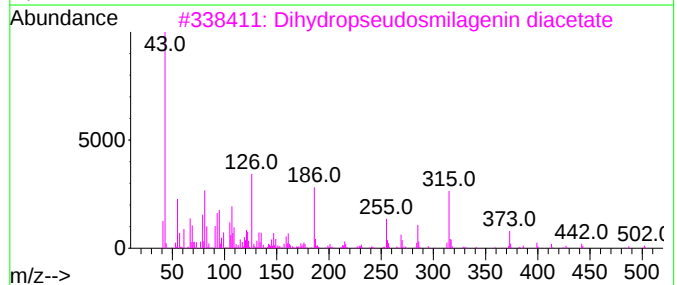
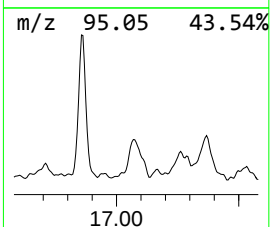
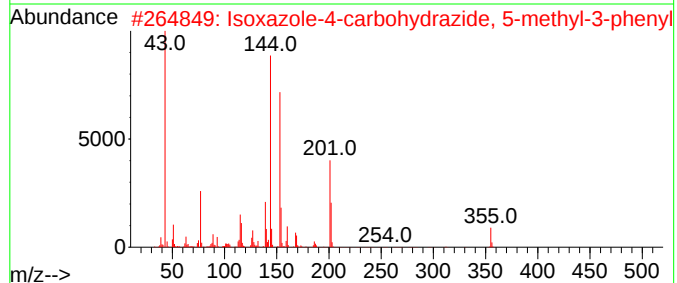
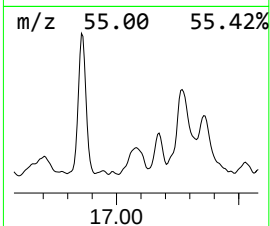
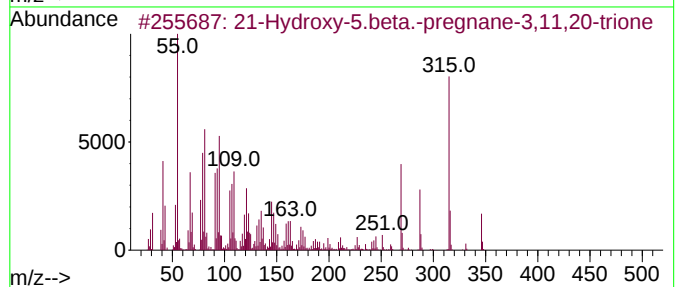
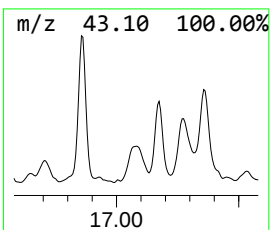
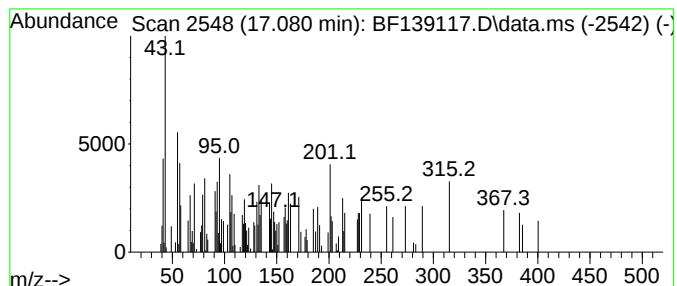
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 17 unknown17.080 Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.080	4.13 ng	120784	Perylene-d12	15.533

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	21-Hydroxy-5.β.-pregnane-3,11...	346	C21H30O4	010417-86-4	10		
2	Isoxazole-4-carbohydrazide, 5-me...	355	C22H17N3O2	1000264-87-1	9		
3	Dihydropseudosmilagenin diacetate	502	C31H50O5	1000255-26-9	9		
4	5-β.-Card-20(22)-enolide, 7-...	418	C23H30O7	022146-03-8	9		
5	Isopropyl N-(3-chloro-4-methoxy...	243	C11H14ClNO3	1000314-78-7	9		



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082224\
Data File : BF139117.D
Acq On : 22 Aug 2024 12:22
Operator : RC/JU
Sample : P3641-04
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
S-908-K1-0.5-1.0-081524

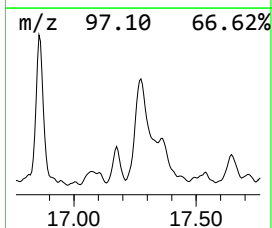
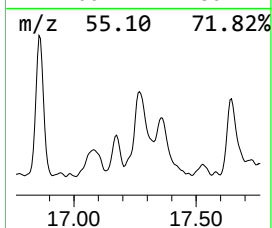
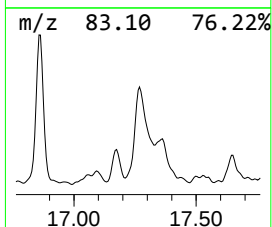
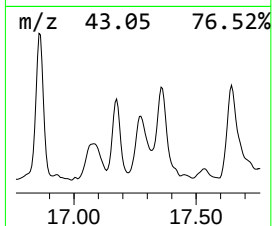
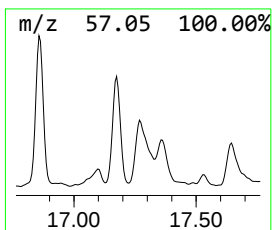
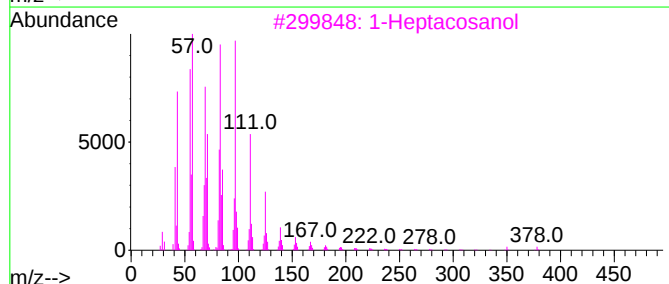
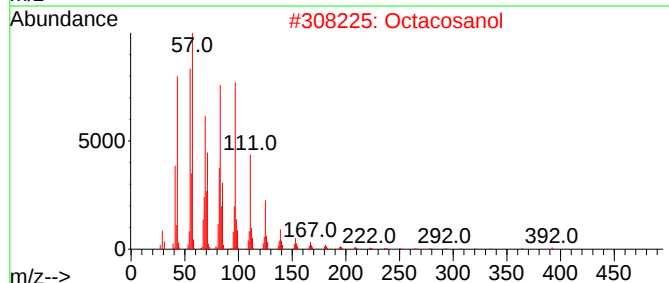
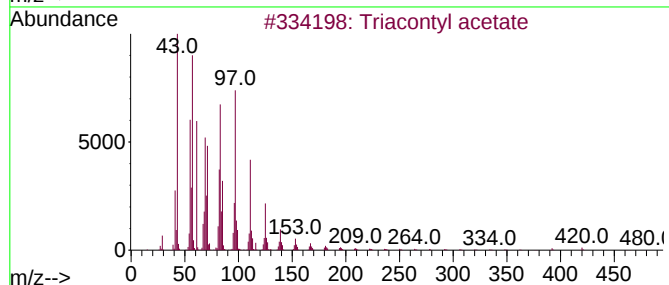
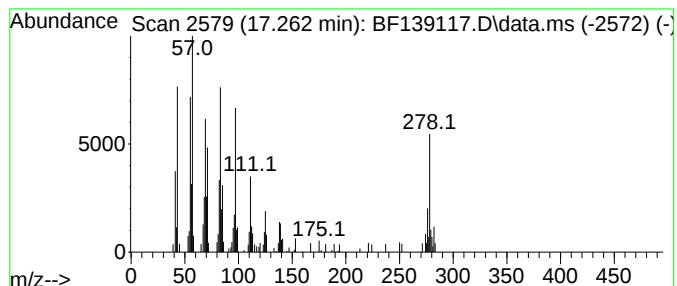
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 18 Triacontyl acetate Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.262	7.42 ng	217057	Perylene-d12	15.533

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Triacontyl acetate	480	C32H64O2	041755-58-2	93
2			Octacosanol	410	C28H58O	000557-61-9	93
3			1-Heptacosanol	396	C27H56O	002004-39-9	91
4			1-Octadecene	252	C18H36	000112-88-9	91
5			Methyl tetratriacontyl ether	509	C35H72O	1000406-30-1	86



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082224\
Data File : BF139117.D
Acq On : 22 Aug 2024 12:22
Operator : RC/JU
Sample : P3641-04
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
S-908-K1-0.5-1.0-081524

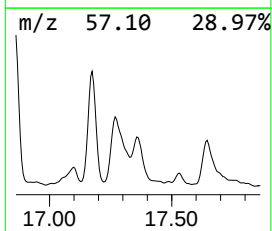
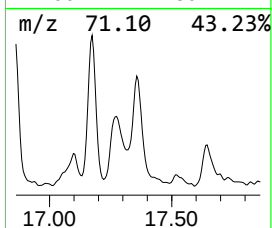
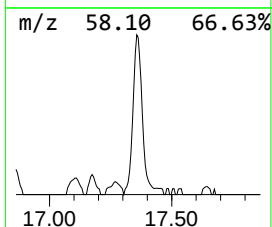
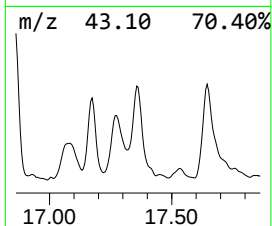
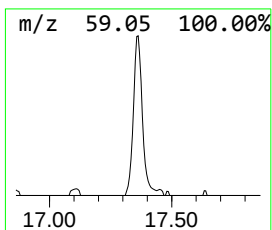
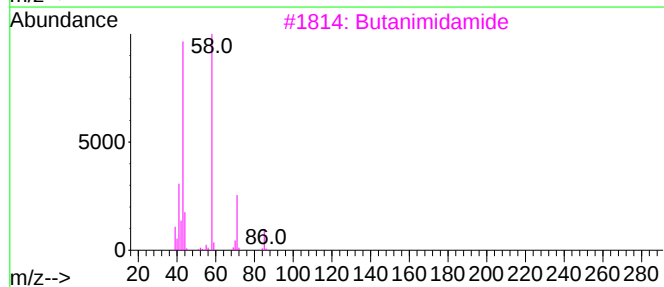
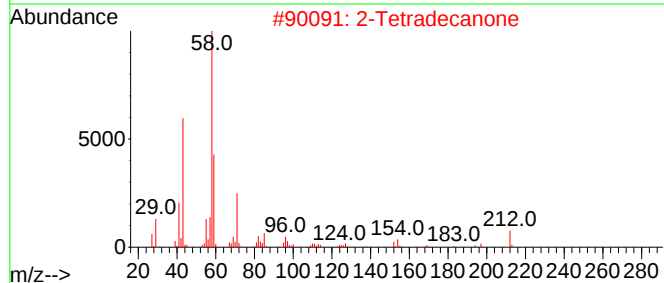
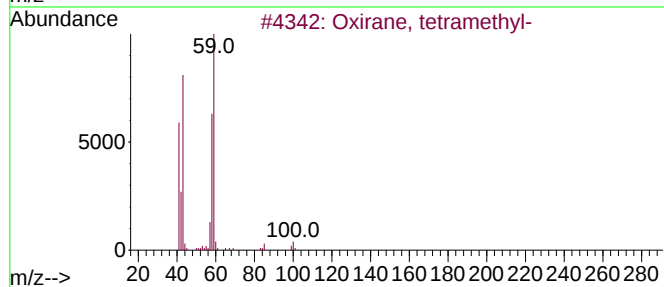
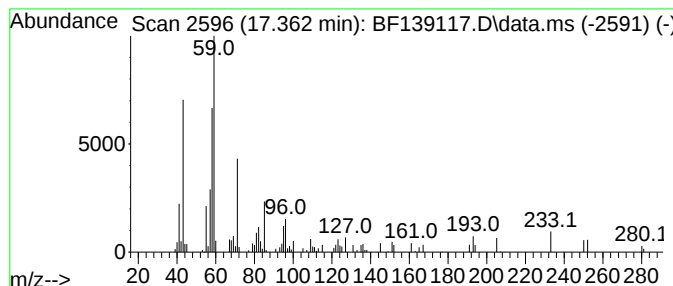
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 19 unknown17.362 Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.362	4.39 ng	128508	Perylene-d12	15.533

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Oxirane, tetramethyl-	100	C6H12O	005076-20-0	43
2		2-Tetradecanone	212	C14H28O	002345-27-9	38
3		Butanimidamide	86	C4H10N2	000107-90-4	35
4		2-Hexadecanone	240	C16H32O	018787-63-8	32
5		Octanal, 7-hydroxy-3,7-dimethyl-	172	C10H20O2	000107-75-5	32



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082224\
Data File : BF139117.D
Acq On : 22 Aug 2024 12:22
Operator : RC/JU
Sample : P3641-04
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
S-908-K1-0.5-1.0-081524

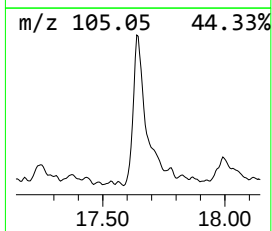
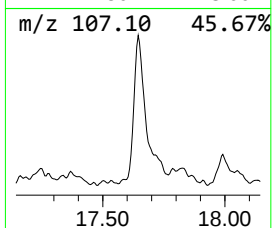
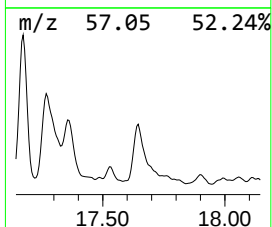
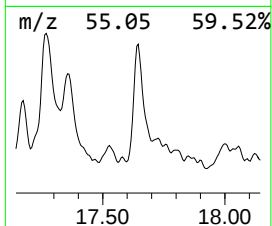
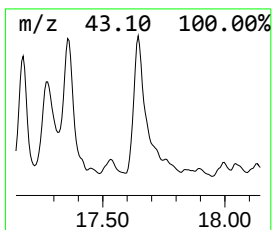
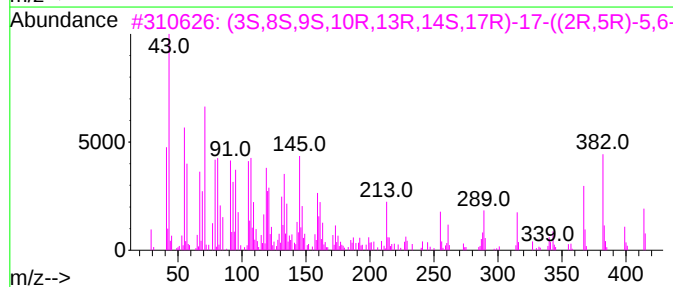
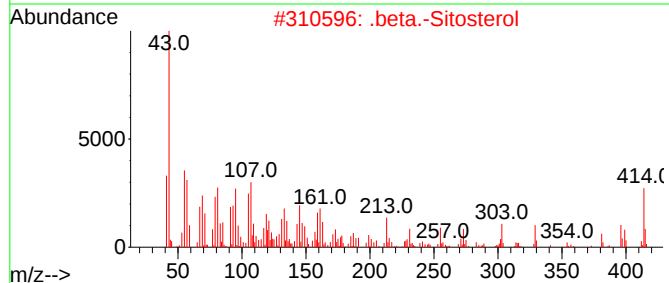
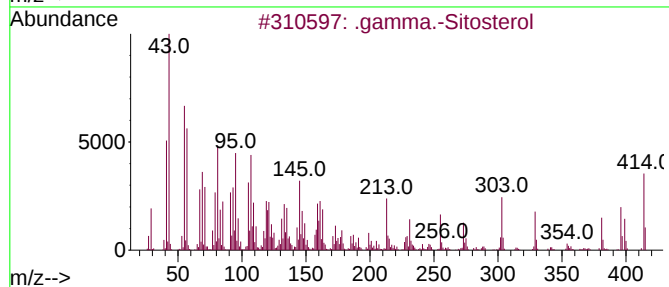
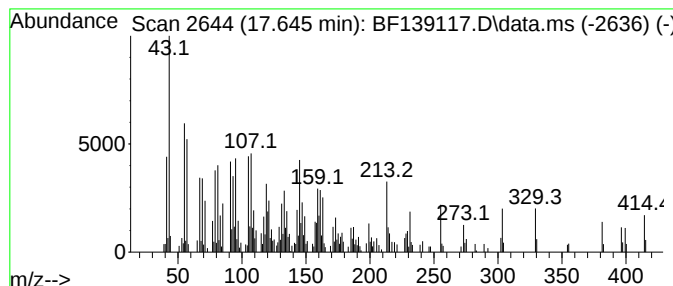
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 20 .gamma.-Sitosterol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.645	15.26 ng	446546	Perylene-d12	15.533

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			.gamma.-Sitosterol	414	C29H50O	000083-47-6	99
2			.beta.-Sitosterol	414	C29H50O	000083-46-5	99
3			(3S,8S,9S,10R,13R,14S,17R)-17-((...)	414	C29H50O	029365-29-5	80
4			Cholest-5-ene, 3-ethoxy-, (3.bet...	414	C29H50O	000986-19-6	64
5			Ergost-7-en-3-ol	400	C28H48O	116179-22-7	56



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082224\
Data File : BF139117.D
Acq On : 22 Aug 2024 12:22
Operator : RC/JU
Sample : P3641-04
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
S-908-K1-0.5-1.0-081524

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF082024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	2.222	54.6	ng	1629570	1	6.898	597310	20.0
2-Pentanone, 4-...	5.116	7.0	ng	210255	1	6.898	597310	20.0
.alpha.-Pinene	6.181	3.9	ng	115236	1	6.898	597310	20.0
Humulene	9.786	3.6	ng	184107	3	9.933	1013260	20.0
n-Hexadecanoic ...	11.945	5.2	ng	295114	4	11.416	1143250	20.0
Cinnamyl cinnamate	13.774	33.5	ng	1635700	5	14.057	977043	20.0
Cyclohexadecane	13.910	6.0	ng	294890	5	14.057	977043	20.0
1-Octadecene	14.539	10.4	ng	508670	5	14.057	977043	20.0
Eicosanal-	14.998	6.0	ng	175415	6	15.533	585119	20.0
Heneicosane	15.198	12.7	ng	369945	6	15.533	585119	20.0
Benzo[e]pyrene	15.404	5.3	ng	154178	6	15.533	585119	20.0
Oxirane, heptad...	15.792	9.7	ng	282732	6	15.533	585119	20.0
Hexacosane	16.039	12.4	ng	361570	6	15.533	585119	20.0
n-Tetracosanol-1	16.092	7.3	ng	212708	6	15.533	585119	20.0
2-Nonadecanone	16.157	3.7	ng	109470	6	15.533	585119	20.0
1,19-Eicosadiene	16.857	9.3	ng	273249	6	15.533	585119	20.0
unknown17.080	17.080	4.1	ng	120784	6	15.533	585119	20.0
Triacetyl acetate	17.262	7.4	ng	217057	6	15.533	585119	20.0
unknown17.362	17.362	4.4	ng	128508	6	15.533	585119	20.0
.gamma.-Sitosterol	17.645	15.3	ng	446546	6	15.533	585119	20.0