

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF112024\
 Data File : BF140521.D
 Acq On : 21 Nov 2024 00:51
 Operator : RC/JU
 Sample : P4860-02
 Misc :
 ALS Vial : 22 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PH2-BOT-001

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-BF111324.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF140521.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.140	3	8	16	rVB	631826	986369	61.39%	4.860%
2	5.093	505	510	519	rVB	19613	29832	1.86%	0.147%
3	5.187	522	526	531	rVB	13671	17284	1.08%	0.085%
4	5.363	551	556	561	rBV	49707	62944	3.92%	0.310%
5	5.504	575	580	602	rVB	965634	1276377	79.43%	6.289%
6	5.728	614	618	624	rVB	12530	16345	1.02%	0.081%
7	6.334	712	721	724	rBV	13125	27906	1.74%	0.138%
8	6.398	729	732	735	rBV	18850	20911	1.30%	0.103%
9	6.475	740	745	746	rVV2	12040	17025	1.06%	0.084%
10	6.510	746	751	757	rVV	915170	1213558	75.53%	5.980%
11	6.557	757	759	765	rVB2	21334	28962	1.80%	0.143%
12	6.698	779	783	791	rVB2	60948	81572	5.08%	0.402%
13	6.816	796	803	808	rBV2	11655	24632	1.53%	0.121%
14	6.875	808	813	819	rVB	306629	389528	24.24%	1.919%
15	6.928	819	822	829	rVB3	20607	31562	1.96%	0.156%
16	6.993	829	833	835	rBV2	11643	17095	1.06%	0.084%
17	7.122	847	855	856	rBV	24944	34749	2.16%	0.171%
18	7.146	856	859	862	rVV2	31236	41801	2.60%	0.206%
19	7.193	862	867	874	rVB3	33505	70052	4.36%	0.345%
20	7.257	874	878	882	rBV3	13575	22349	1.39%	0.110%
21	7.434	899	908	917	rBV	603818	851495	52.99%	4.196%
22	7.616	935	939	941	rBV	17938	21683	1.35%	0.107%
23	7.663	945	947	956	rVB2	23810	42142	2.62%	0.208%
24	7.769	958	965	967	rBV5	8867	17048	1.06%	0.084%
25	7.893	979	986	990	rBV3	28298	47211	2.94%	0.233%
26	8.151	1023	1030	1037	rBV	288012	435738	27.12%	2.147%
27	8.240	1042	1045	1052	rVB2	12813	19951	1.24%	0.098%
28	8.563	1097	1100	1112	rVB2	15854	28764	1.79%	0.142%
29	8.734	1125	1129	1134	rVB2	19407	24244	1.51%	0.119%
30	8.869	1148	1152	1159	rVB2	27042	35347	2.20%	0.174%
31	8.963	1164	1168	1175	rVB	12594	18120	1.13%	0.089%
32	9.169	1200	1203	1207	rVB	14123	16882	1.05%	0.083%
33	9.228	1207	1213	1222	rBV	1076137	1372303	85.40%	6.762%
34	9.304	1222	1226	1230	rBV	23803	32134	2.00%	0.158%
35	9.563	1263	1270	1273	rBV3	18550	37647	2.34%	0.186%
36	9.622	1276	1280	1287	rVB3	21697	39139	2.44%	0.193%

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37	9.834	1310	1316	1320	rBV2	21842	32760	2.04%	0.161%
38	9.910	1323	1329	1342	rVB	317572	437841	27.25%	2.157%
39	10.157	1367	1371	1375	rBV4	12357	17113	1.07%	0.084%
40	10.334	1394	1401	1404	rBV2	27035	44229	2.75%	0.218%
41	10.428	1413	1417	1421	rBV	25695	35043	2.18%	0.173%
42	10.551	1434	1438	1445	rVB2	21558	39297	2.45%	0.194%
43	10.622	1445	1450	1455	rBV	74789	99274	6.18%	0.489%
44	10.698	1458	1463	1473	rVV	626588	835727	52.01%	4.118%
45	10.816	1478	1483	1490	rVB2	67020	125968	7.84%	0.621%
46	10.881	1490	1494	1495	rBV2	22535	26683	1.66%	0.131%
47	10.910	1496	1499	1503	rVV3	14752	20760	1.29%	0.102%
48	11.028	1516	1519	1522	rVB	16165	17016	1.06%	0.084%
49	11.098	1528	1531	1534	rBV	12323	16151	1.01%	0.080%
50	11.169	1540	1543	1549	rVB	39146	47345	2.95%	0.233%
51	11.257	1554	1558	1560	rVV	32616	47003	2.93%	0.232%
52	11.281	1560	1562	1568	rVB2	45636	62429	3.89%	0.308%
53	11.398	1577	1582	1591	rBV	360464	512200	31.88%	2.524%
54	11.633	1620	1622	1626	rBV2	12742	16772	1.04%	0.083%
55	11.681	1627	1630	1634	rVB	27055	33310	2.07%	0.164%
56	11.922	1667	1671	1681	rBV	248963	414949	25.82%	2.045%
57	12.092	1697	1700	1704	rVB	25943	30431	1.89%	0.150%
58	12.339	1738	1742	1746	rBV	126352	168919	10.51%	0.832%
59	12.480	1763	1766	1770	rVB	41066	50281	3.13%	0.248%
60	12.622	1786	1790	1791	rBV	36112	48247	3.00%	0.238%
61	12.651	1791	1795	1800	rVV	466955	607191	37.79%	2.992%
62	12.710	1801	1805	1812	rVV	61365	113030	7.03%	0.557%
63	12.851	1825	1829	1835	rBV2	82114	105189	6.55%	0.518%
64	12.986	1846	1852	1859	rVB	1240462	1606820	100.00%	7.917%
65	13.122	1872	1875	1880	rVB	88355	103639	6.45%	0.511%
66	13.210	1886	1890	1894	rBV	124565	156951	9.77%	0.773%
67	13.551	1944	1948	1955	rBV	192338	249137	15.50%	1.228%
68	13.845	1994	1998	2001	rBV	281688	366847	22.83%	1.808%
69	13.880	2001	2004	2018	rVB	273857	444244	27.65%	2.189%
70	14.016	2024	2027	2029	rBV	165485	193078	12.02%	0.951%
71	14.045	2029	2032	2041	rVB	260985	373381	23.24%	1.840%
72	14.174	2051	2054	2056	rBV	169023	223505	13.91%	1.101%
73	14.204	2056	2059	2064	rVB2	298479	542172	33.74%	2.671%
74	14.510	2107	2111	2116	rBV	290077	390941	24.33%	1.926%
75	14.821	2160	2164	2172	rVB	247748	342321	21.30%	1.687%
76	14.898	2173	2177	2186	rVB	147747	207831	12.93%	1.024%

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77	15.163	2218	2222	2228	rVB	235866	339787	21.15%	1.674%
78	15.551	2282	2288	2295	rVB2	261141	464920	28.93%	2.291%
79	15.998	2360	2364	2370	rVB	113577	187328	11.66%	0.923%
80	16.263	2402	2409	2432	rVB3	286809	946693	58.92%	4.665%
81	16.463	2436	2443	2449	rBV2	674279	1296904	80.71%	6.390%
82	17.204	2565	2569	2575	rBV4	43880	92682	5.77%	0.457%
83	17.674	2643	2649	2661	rVB2	124105	309715	19.28%	1.526%

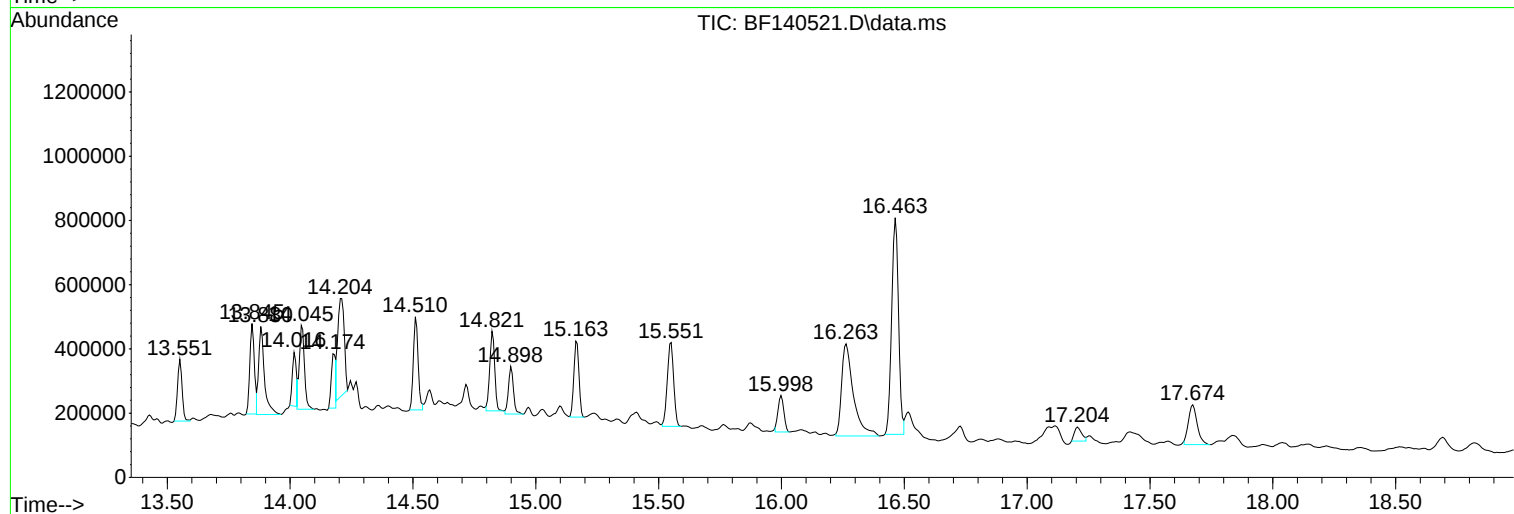
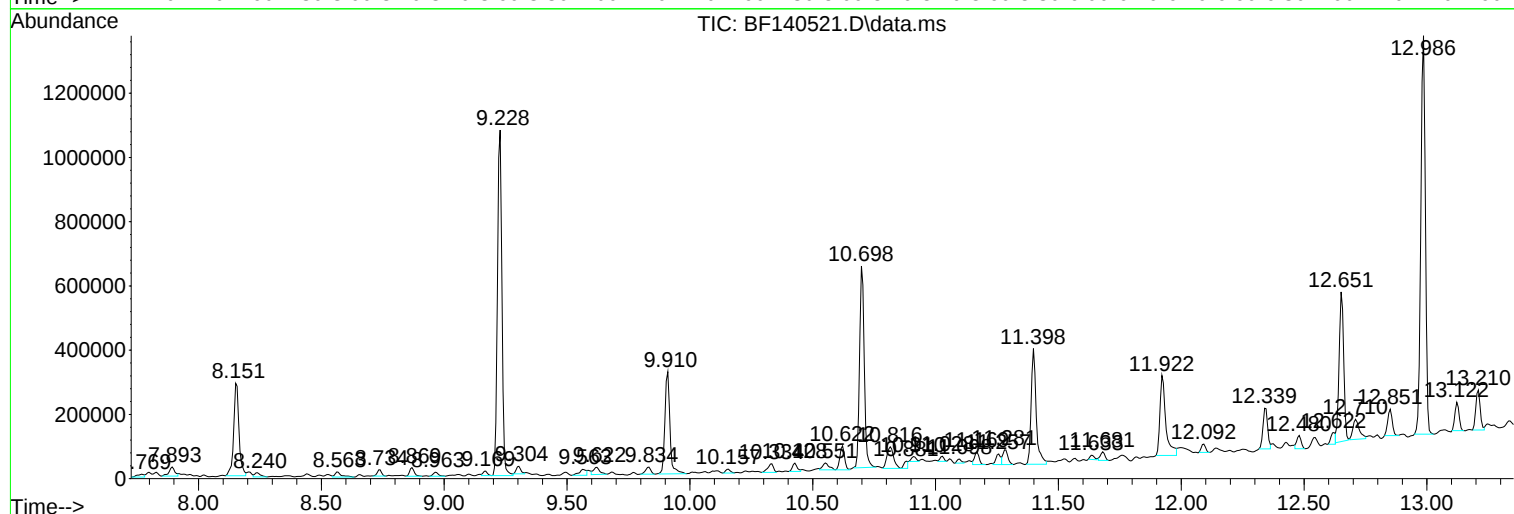
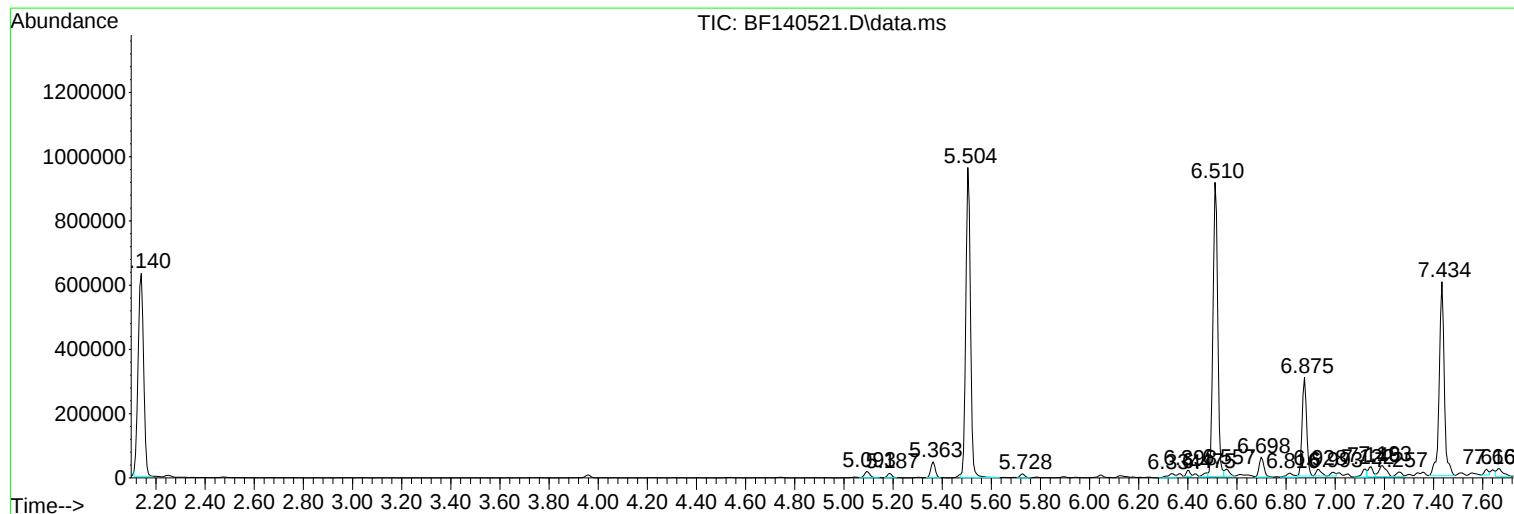
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Instrument :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF111324.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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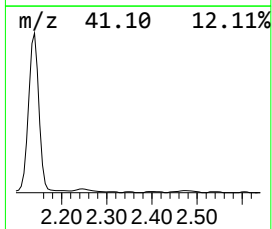
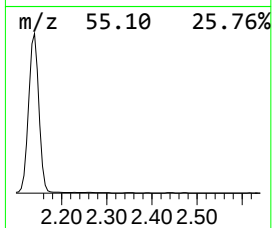
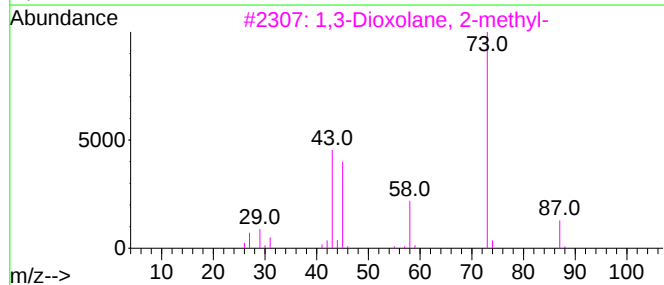
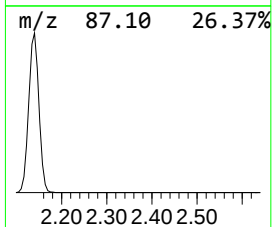
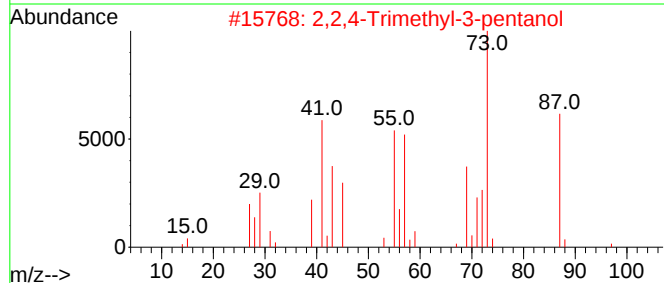
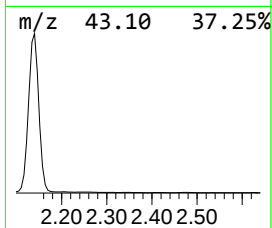
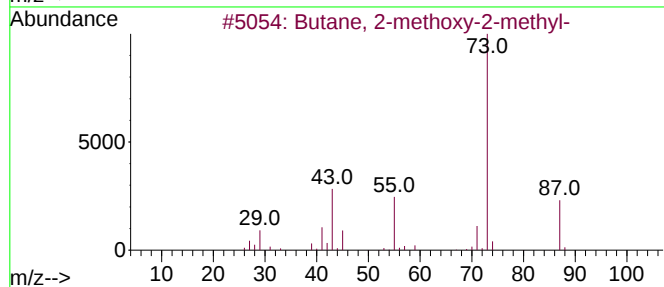
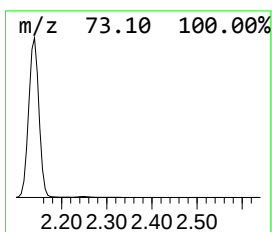
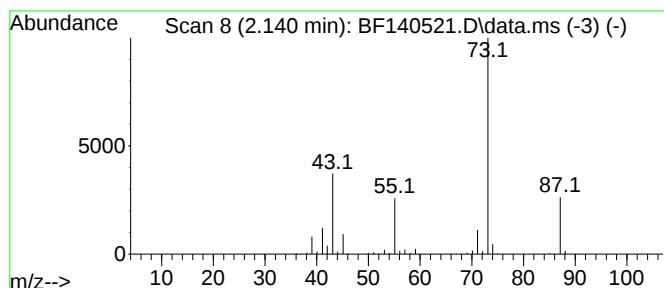
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF111324.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.140	50.64 ng	986369	1,4-Dichlorobenzene-d4	6.875

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
4			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17
5			Silane, tetramethyl-	88	C4H12Si	000075-76-3	12



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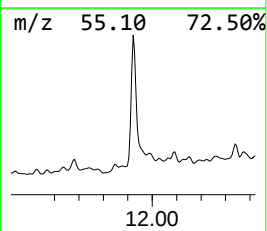
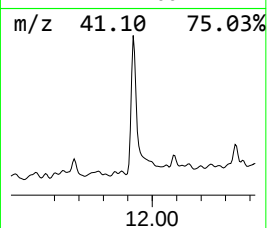
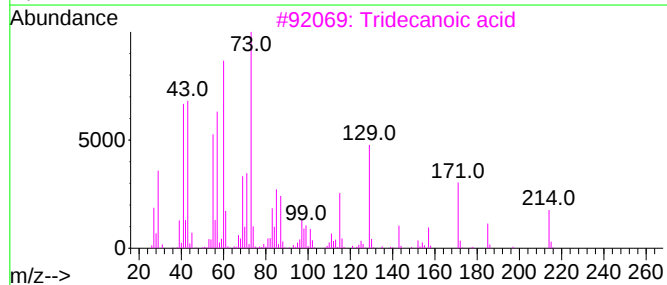
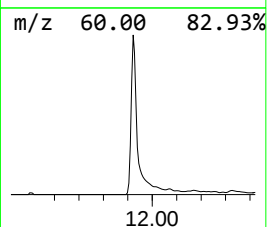
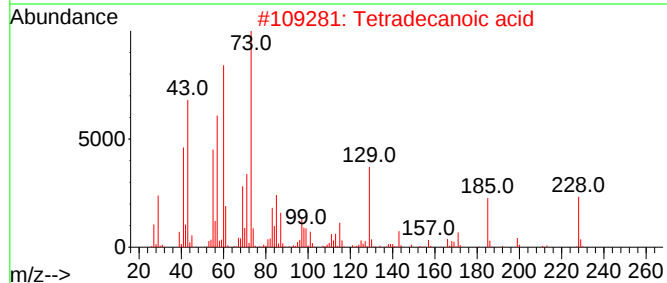
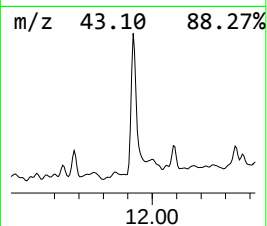
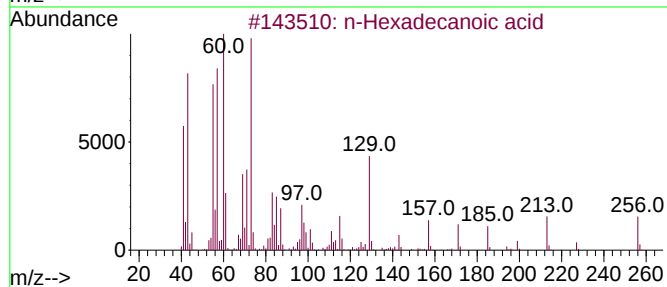
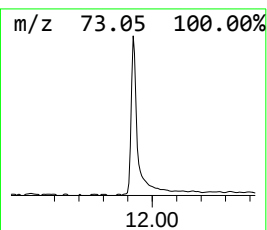
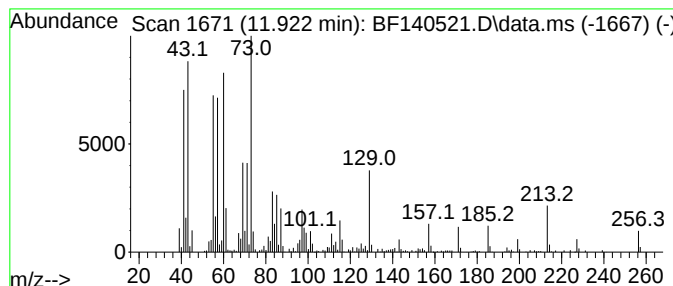
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 n-Hexadecanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.922	16.20 ng	414949	Phenanthrene-d10	11.398

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	94
3			Tridecanoic acid	214	C13H26O2	000638-53-9	91
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	91
5			n-Decanoic acid	172	C10H20O2	000334-48-5	76



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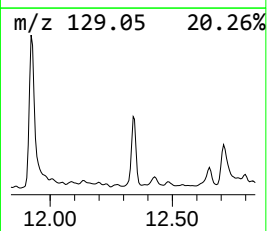
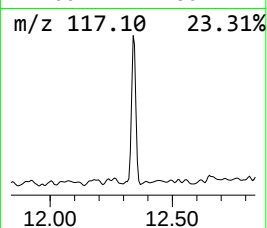
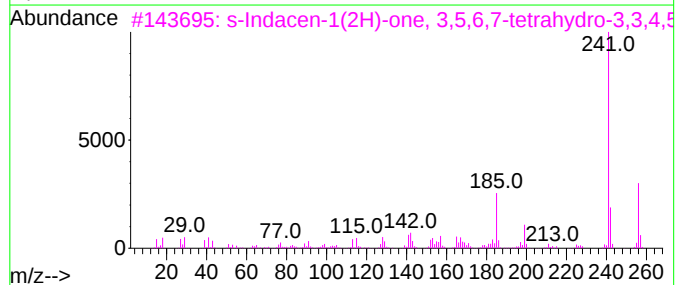
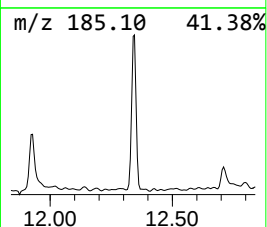
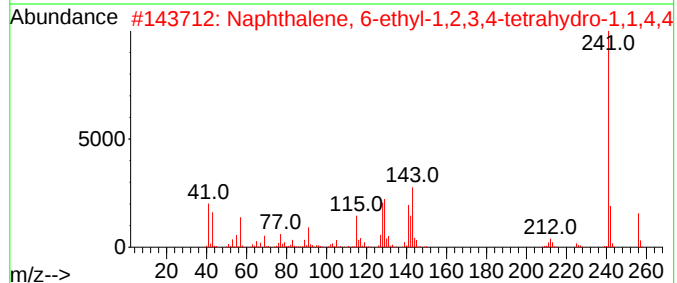
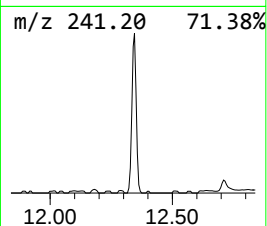
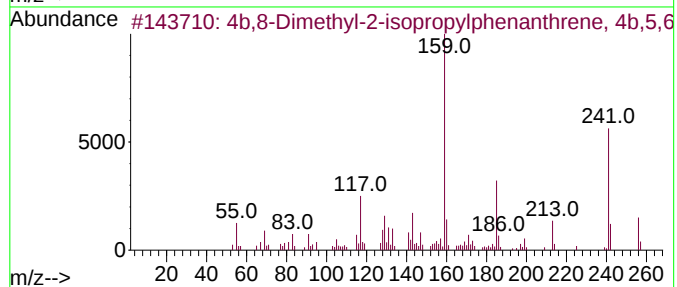
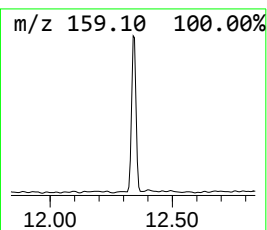
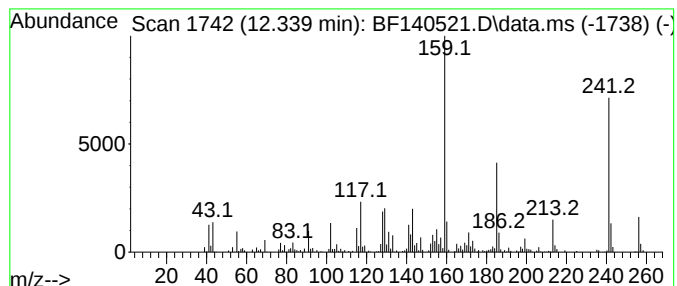
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 4b,8-Dimethyl-2-isopropylph... Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.339	6.60 ng	168919	Phenanthrene-d10	11.398

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			4b,8-Dimethyl-2-isopropylphenant...	256	C19H28	1000197-14-1	98
2			Naphthalene, 6-ethyl-1,2,3,4-tet...	256	C19H28	301643-35-6	74
3			s-Indacen-1(2H)-one, 3,5,6,7-tet...	256	C18H24O	038754-94-8	56
4			Pyrazol-4-amine, 1-(3,4-dichloro...	241	C10H9Cl2N3	1000273-77-4	46
5			1-[[3-(Trifluoromethyl)phenyl]me...	241	C11H10F3N3	1002033-51-3	43



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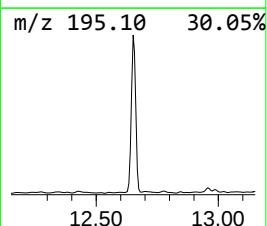
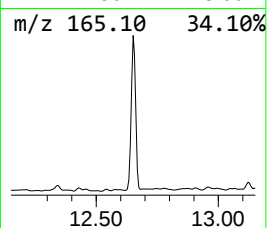
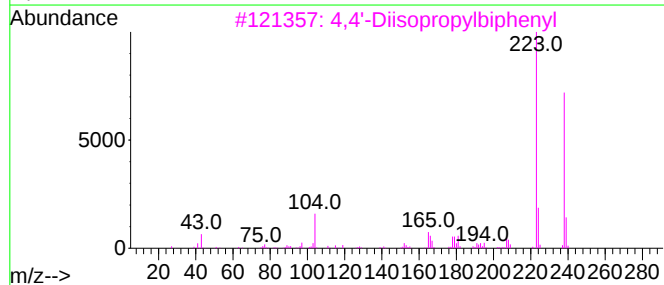
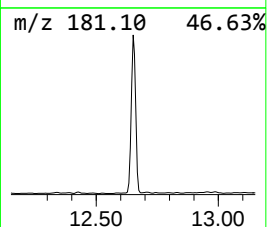
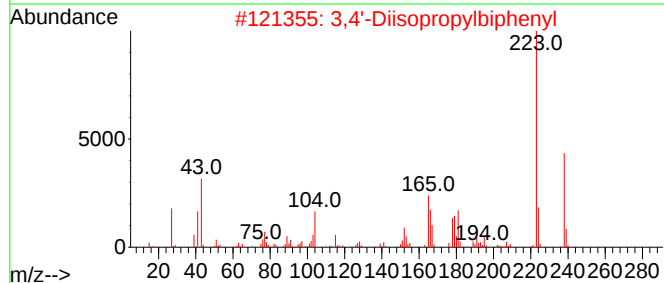
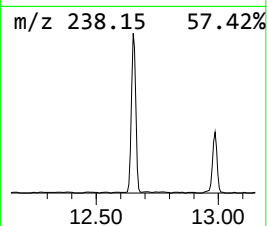
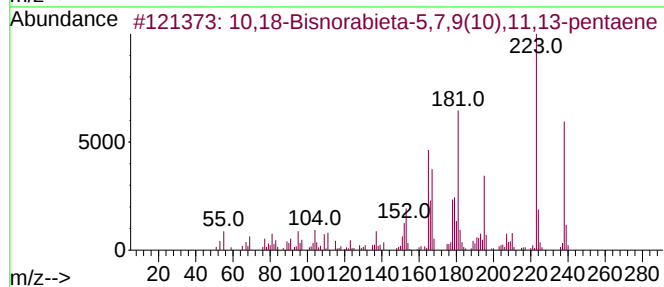
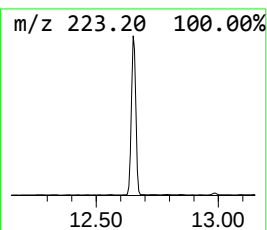
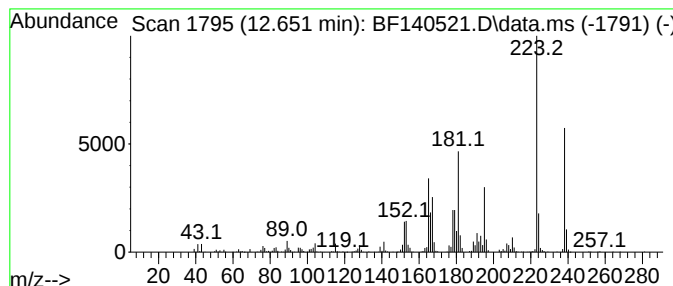
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ClientSampleId :
PH2-BOT-001

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF111324.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 10,18-Bisnorabieta-5,7,9(10... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.651	23.71 ng	607191	Phenanthrene-d10	11.398	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	10,18-Bisnorabieta-5,7,9(10),11,...	238	C18H22	006566-19-4	99
2	3,4'-Diisopropylbiphenyl	238	C18H22	061434-46-6	90
3	4,4'-Diisopropylbiphenyl	238	C18H22	018970-30-4	55
4	4-tert-Butylbenzenethiol, S-trim...	238	C13H22SSi	123045-43-2	46
5	2-Propenoic acid, 3-(3,4,5-trime...	238	C12H14O5	000090-50-6	46



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF112024\
Data File : BF140521.D
Acq On : 21 Nov 2024 00:51
Operator : RC/JU
Sample : P4860-02
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PH2-BOT-001

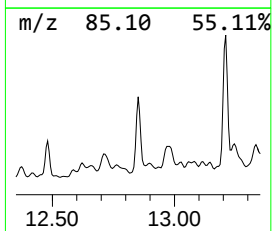
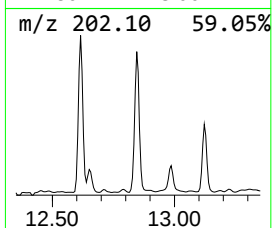
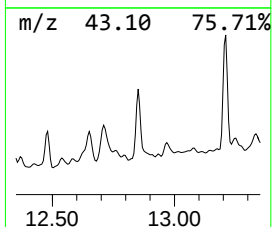
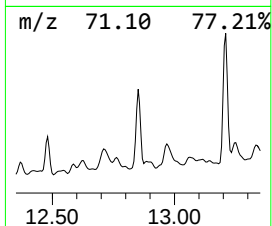
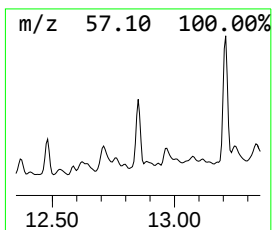
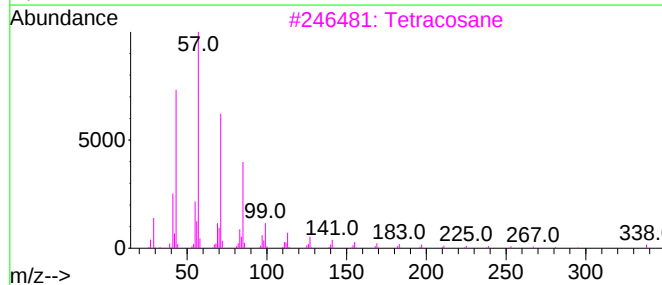
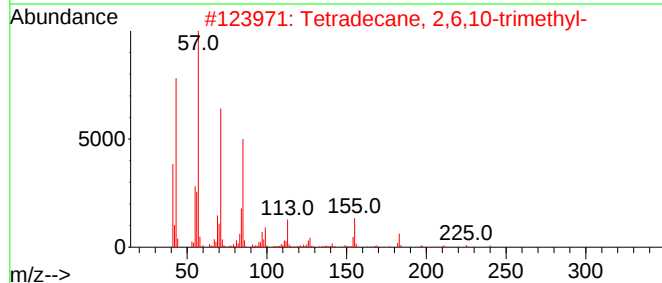
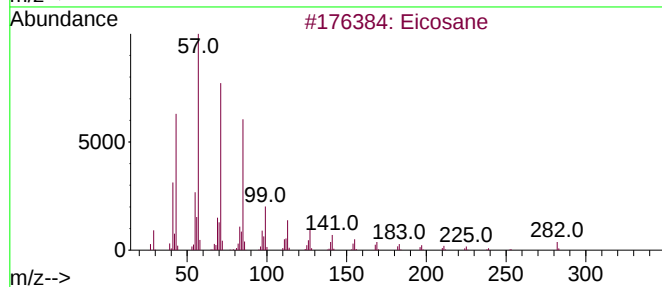
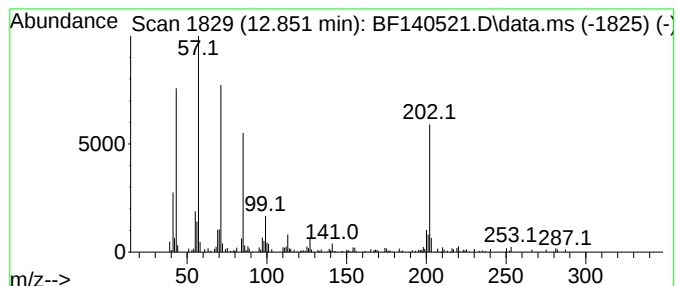
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Eicosane Concentration Rank 19

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.851	5.63 ng	105189	Chrysene-d12	14.045

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Eicosane	282	C20H42	000112-95-8	70
2			Tetradecane, 2,6,10-trimethyl-	240	C17H36	014905-56-7	62
3			Tetracosane	338	C24H50	000646-31-1	62
4			Nonadecane	268	C19H40	000629-92-5	58
5			Pentadecane	212	C15H32	000629-62-9	58



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF112024\
Data File : BF140521.D
Acq On : 21 Nov 2024 00:51
Operator : RC/JU
Sample : P4860-02
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PH2-BOT-001

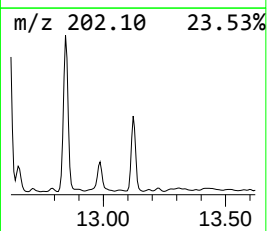
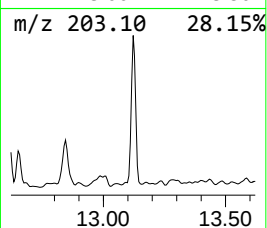
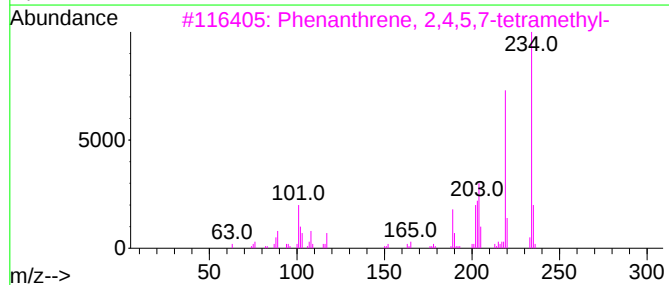
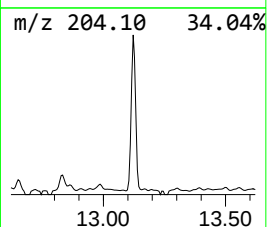
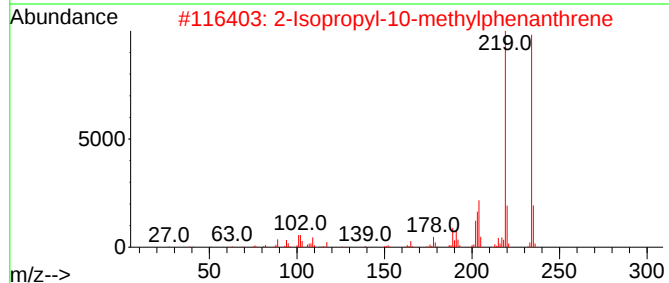
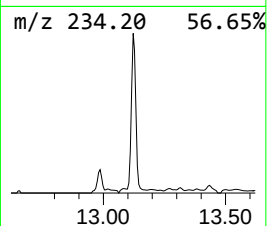
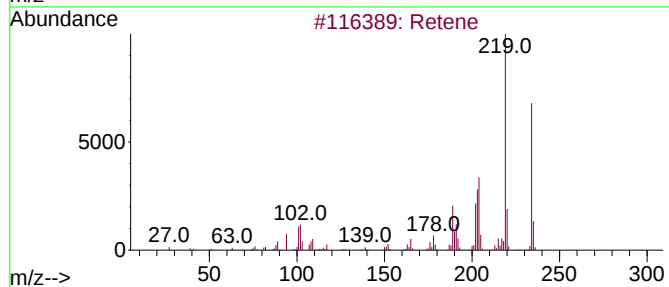
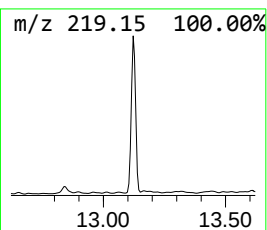
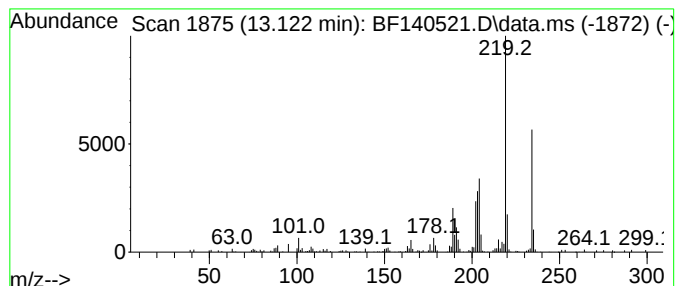
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Retene Concentration Rank 20

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.122	5.55 ng	103639	Chrysene-d12	14.045

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Retene	234	C18H18	000483-65-8	95
2			2-Isopropyl-10-methylphenanthrene	234	C18H18	066552-97-4	94
3			Phenanthrene, 2,4,5,7-tetramethyl-	234	C18H18	007396-38-5	64
4			Ethanone, 1-(4,6-dihydroxy-2,3,5...	234	C13H14O4	021987-07-5	49
5			2-[[1-(4-Methylphenyl)ethylidene...	234	C16H14N2	1000326-46-0	49



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF112024\
Data File : BF140521.D
Acq On : 21 Nov 2024 00:51
Operator : RC/JU
Sample : P4860-02
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PH2-BOT-001

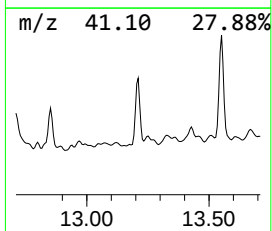
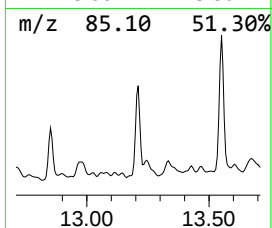
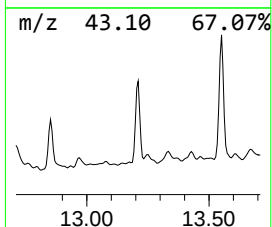
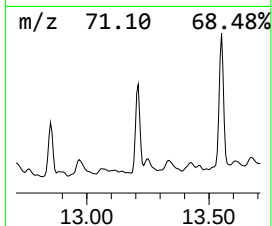
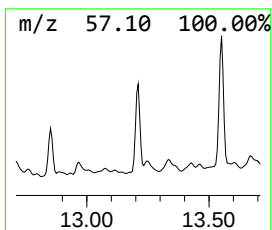
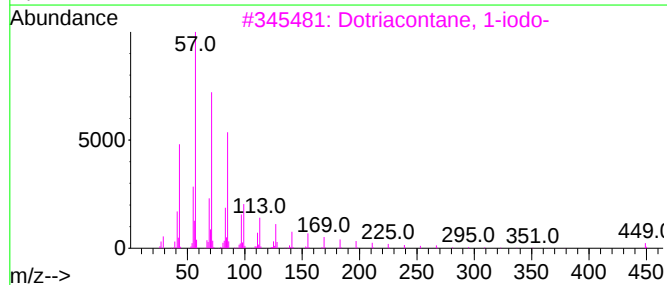
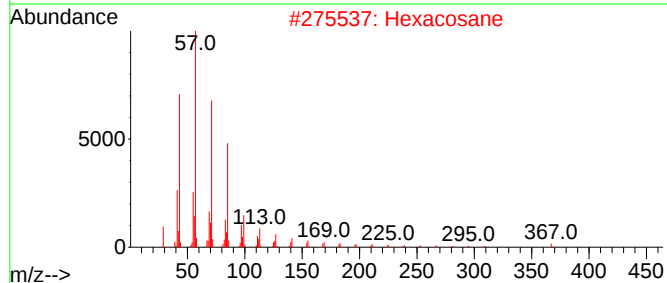
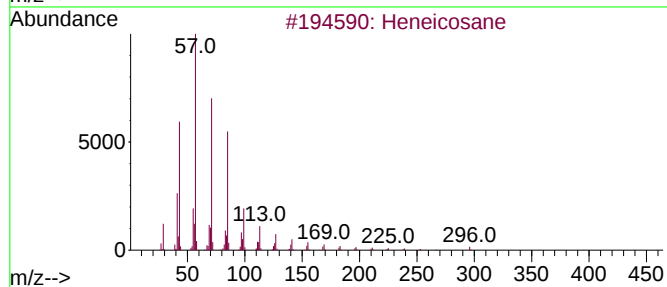
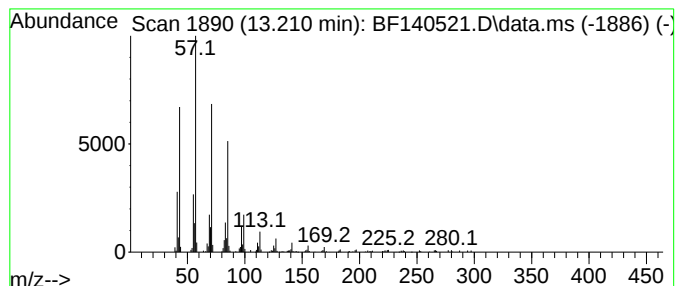
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Heneicosane Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.210	8.41 ng	156951	Chrysene-d12	14.045

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heneicosane	296	C21H44	000629-94-7	91
2			Hexacosane	366	C26H54	000630-01-3	91
3			Dotriacontane, 1-iodo-	576	C32H65I	1000406-32-4	91
4			Octacosane	394	C28H58	000630-02-4	91
5			Eicosane, 7-hexyl-	366	C26H54	055333-99-8	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF112024\
Data File : BF140521.D
Acq On : 21 Nov 2024 00:51
Operator : RC/JU
Sample : P4860-02
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PH2-BOT-001

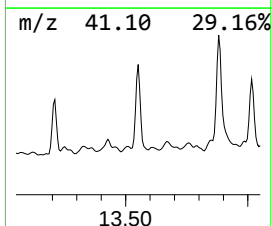
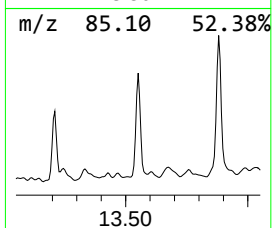
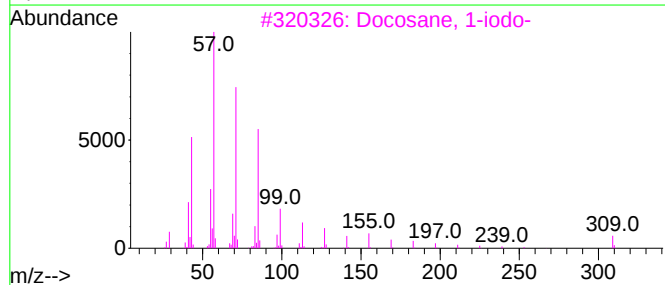
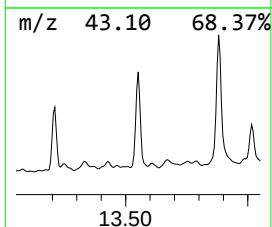
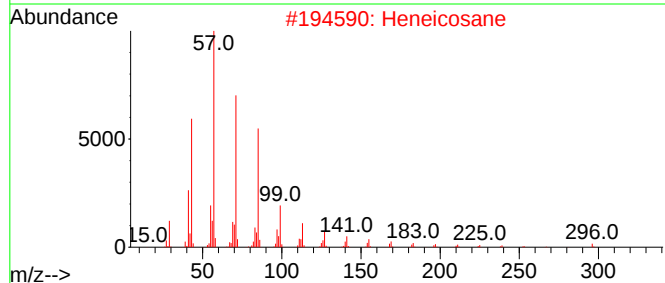
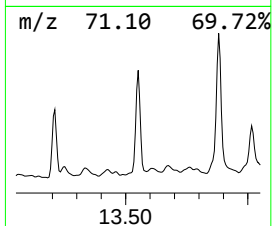
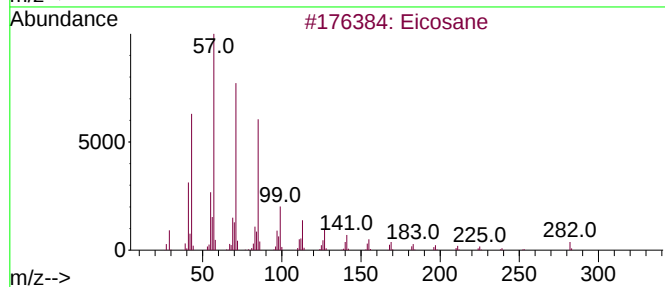
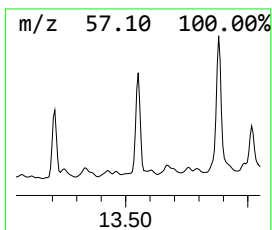
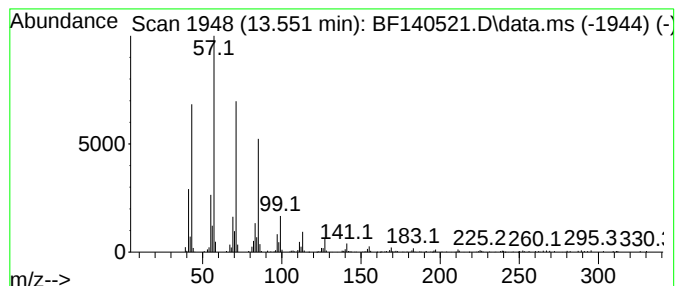
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Docosane, 1-iodo- Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.551	13.34 ng	249137	Chrysene-d12	14.045

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Eicosane	282	C20H42	000112-95-8	94
2			Heneicosane	296	C21H44	000629-94-7	91
3			Docosane, 1-iodo-	436	C22H45I	1000406-31-9	91
4			Heptacosane	380	C27H56	000593-49-7	91
5			Eicosane, 7-hexyl-	366	C26H54	055333-99-8	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF112024\
Data File : BF140521.D
Acq On : 21 Nov 2024 00:51
Operator : RC/JU
Sample : P4860-02
Misc :
ALS Vial : 22 Sample Multiplier: 1

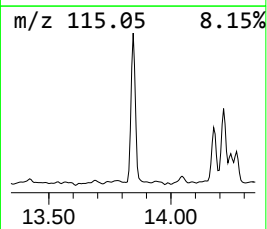
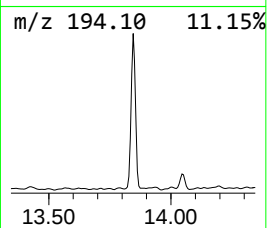
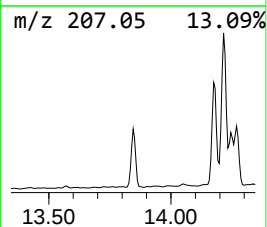
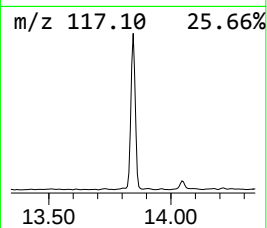
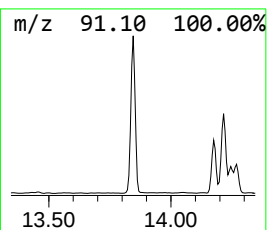
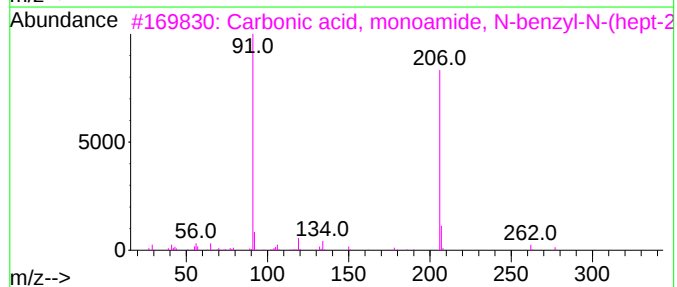
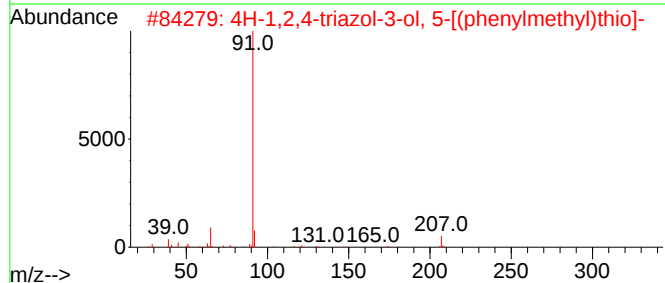
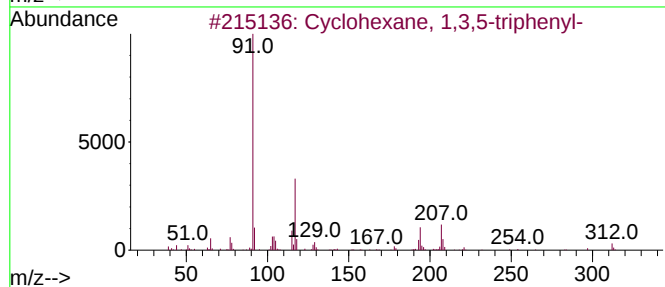
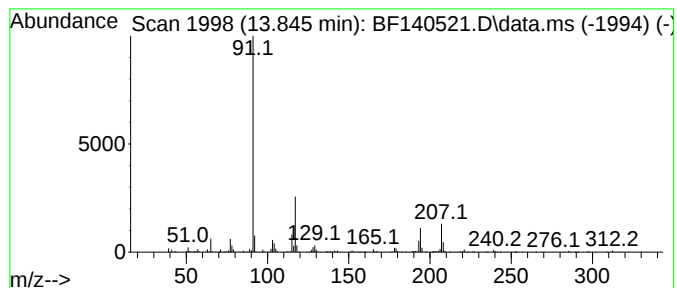
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Cyclohexane, 1,3,5-triphenyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD		R.T.	
13.845	19.65 ng	366847	Chrysene-d12		14.045	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Cyclohexane, 1,3,5-triphenyl-		312	C24H24	028336-57-4	80
2	4H-1,2,4-triazol-3-ol, 5-[(pheny...		207	C9H9N3OS	1010400-54-3	35
3	Carbonic acid, monoamide, N-benz...		277	C17H27NO2	1000450-65-0	16
4	(R)-(1-Cyclopentylpropane-1,3-di...		264	C20H24	1402851-74-4	16
5	Carbonic acid, monoamide, N-benz...		207	C12H17NO2	1000451-48-5	16



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF112024\
Data File : BF140521.D
Acq On : 21 Nov 2024 00:51
Operator : RC/JU
Sample : P4860-02
Misc :
ALS Vial : 22 Sample Multiplier: 1

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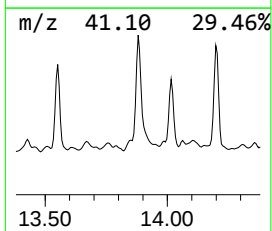
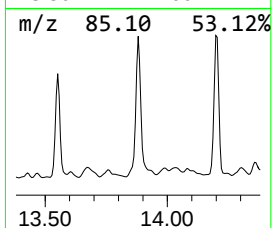
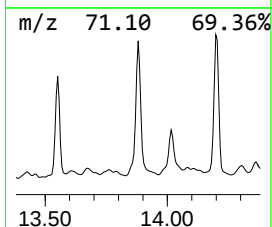
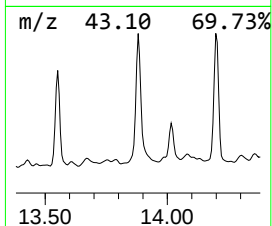
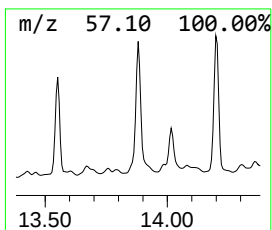
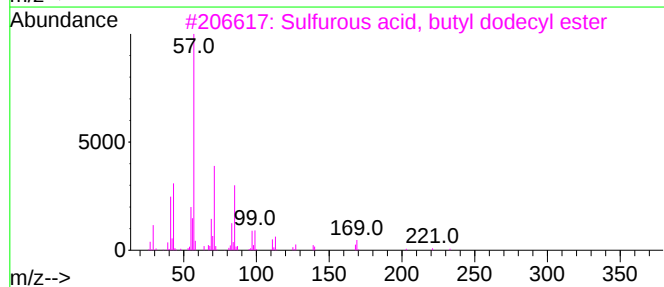
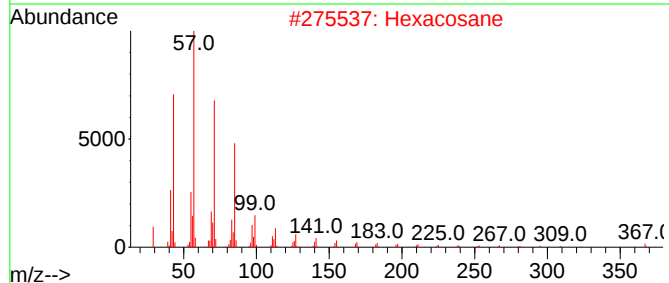
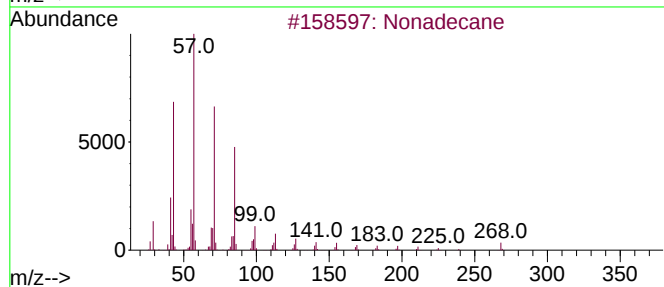
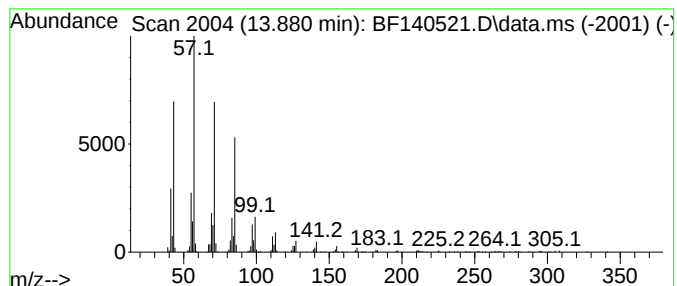
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Nonadecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.880	23.80 ng	444244	Chrysene-d12	14.045

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Nonadecane	268	C19H40	000629-92-5	93
2		Hexacosane	366	C26H54	000630-01-3	91
3		Sulfurous acid, butyl dodecyl ester	306	C16H34O3S	1000309-17-9	91
4		Heneicosane	296	C21H44	000629-94-7	91
5		Heptacosane	380	C27H56	000593-49-7	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF112024\
Data File : BF140521.D
Acq On : 21 Nov 2024 00:51
Operator : RC/JU
Sample : P4860-02
Misc :
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ClientSampleId :
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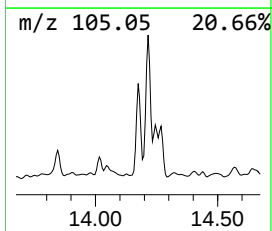
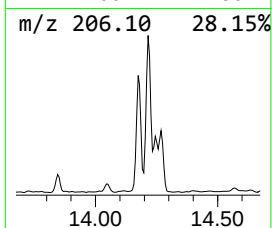
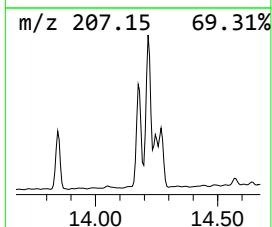
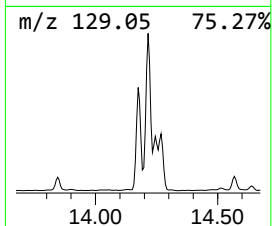
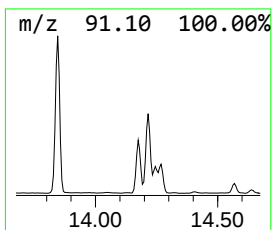
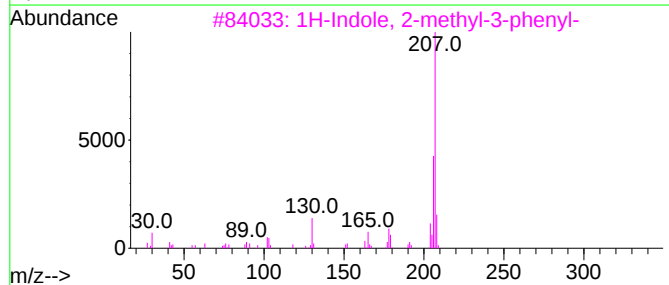
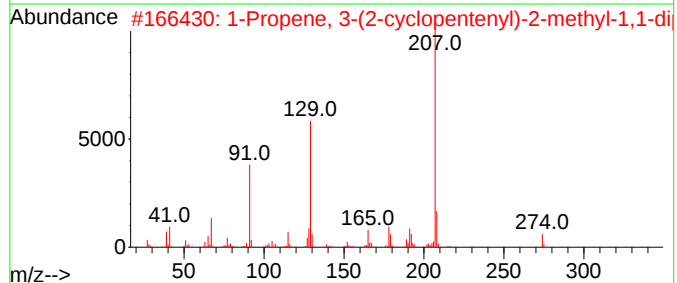
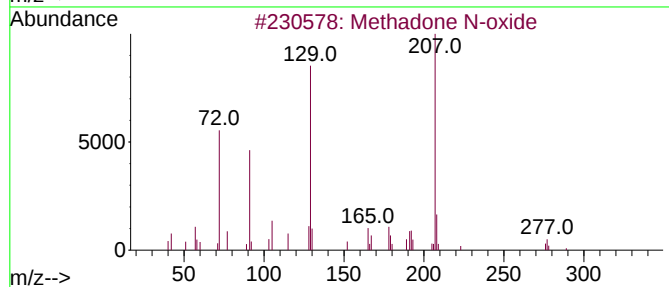
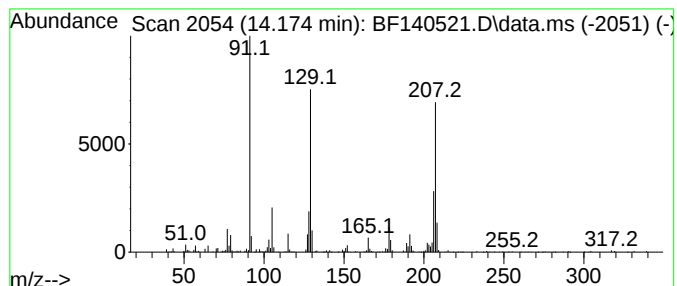
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Methadone N-oxide Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.175	11.97 ng	223505	Chrysene-d12	14.045

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Methadone N-oxide	325	C21H27NO2	1000120-80-7	64
2			1-Propene, 3-(2-cyclopentenyl)-2...	274	C21H22	1010154-23-3	53
3			1H-Indole, 2-methyl-3-phenyl-	207	C15H13N	004757-69-1	38
4			1H-Indole, 1-methyl-2-phenyl-	207	C15H13N	003558-24-5	38
5			4-Methyl-3-phenyl-1H-indole	207	C15H13N	180271-54-9	38



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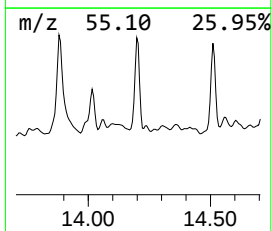
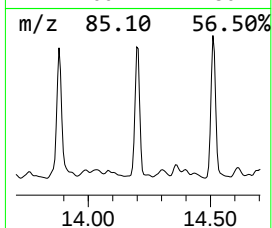
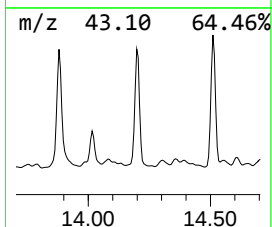
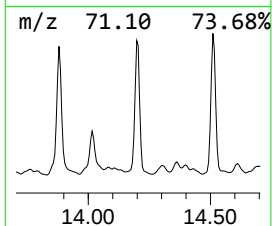
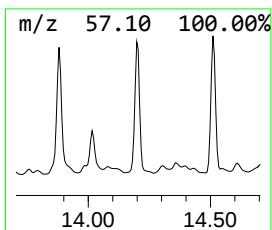
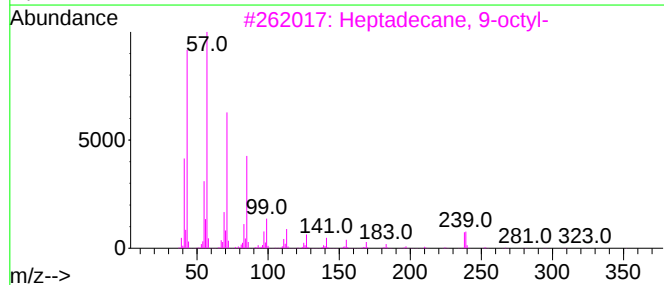
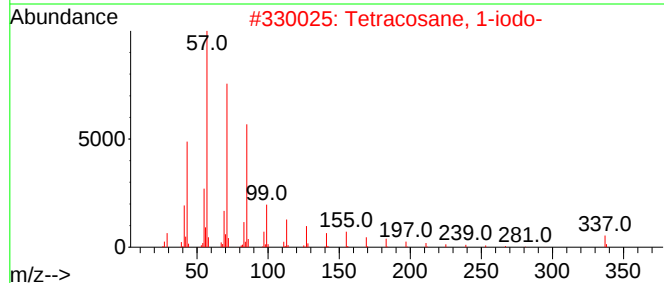
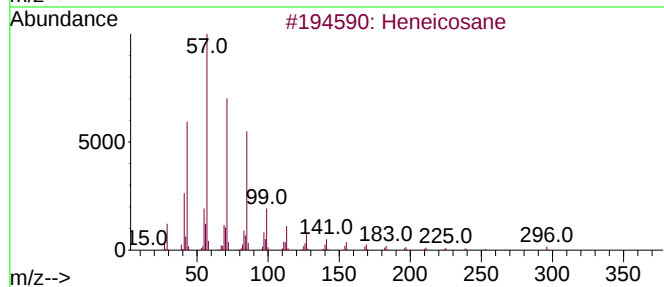
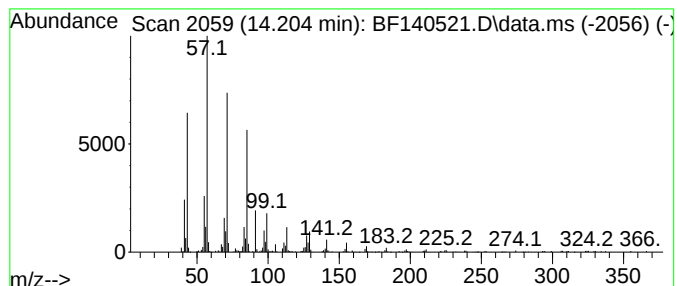
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Tetracosane, 1-iodo- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.204	29.04 ng	542172	Chrysene-d12	14.045	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	90
2	Tetracosane, 1-iodo-	464	C24H49I	1000406-32-0	90
3	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	87
4	Tetracosane	338	C24H50	000646-31-1	87
5	Docosane, 1-iodo-	436	C22H45I	1000406-31-9	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF112024\
Data File : BF140521.D
Acq On : 21 Nov 2024 00:51
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Misc :
ALS Vial : 22 Sample Multiplier: 1

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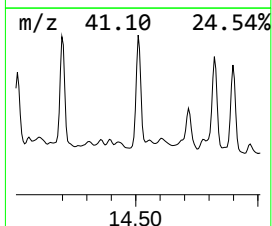
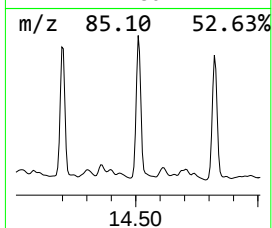
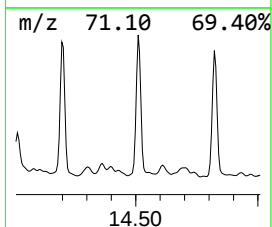
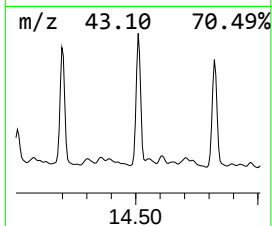
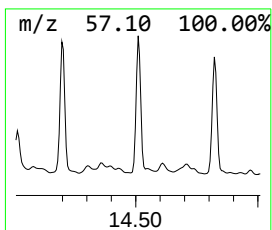
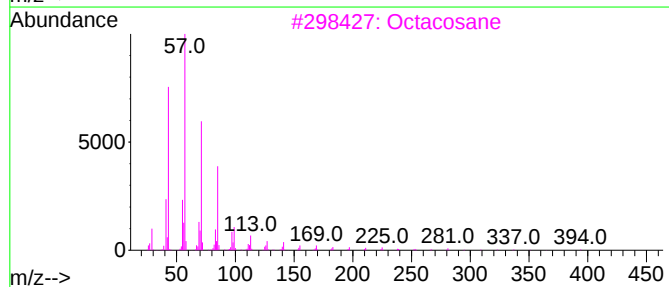
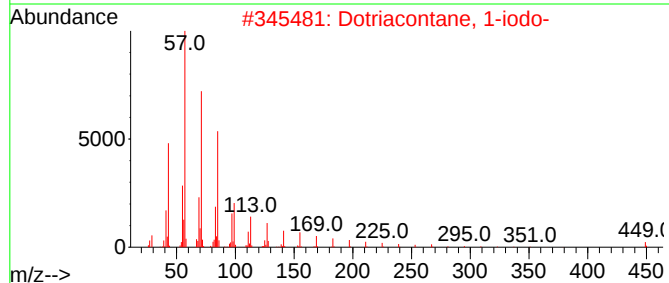
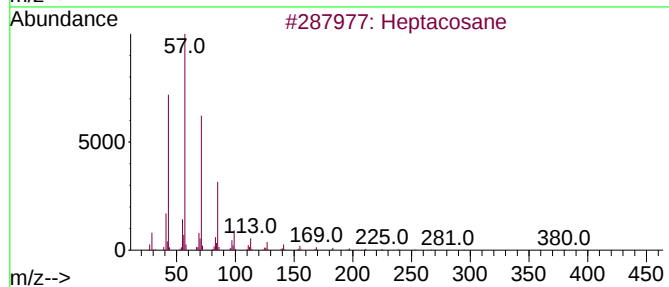
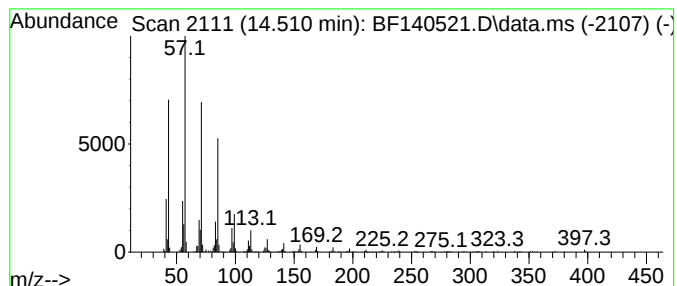
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 13 Heptacosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.510	20.94 ng	390941	Chrysene-d12	14.045

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptacosane	380	C27H56	000593-49-7	95
2			Dotriacontane, 1-iodo-	576	C32H65I	1000406-32-4	91
3			Octacosane	394	C28H58	000630-02-4	91
4			Heneicosane	296	C21H44	000629-94-7	91
5			Octacosane, 1-iodo-	520	C28H57I	1000406-32-2	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF112024\
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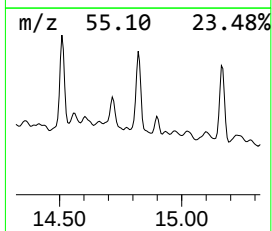
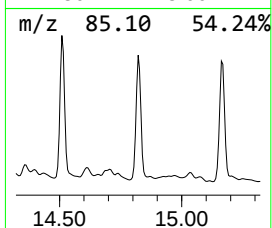
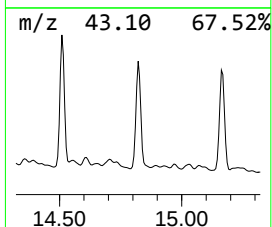
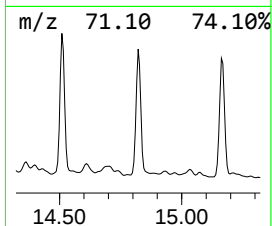
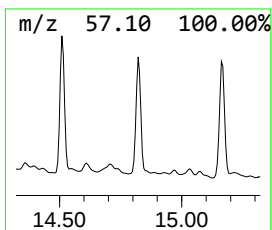
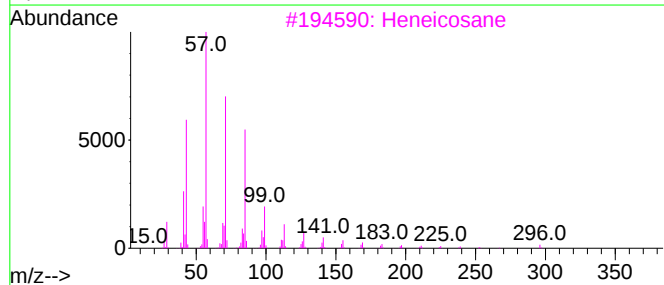
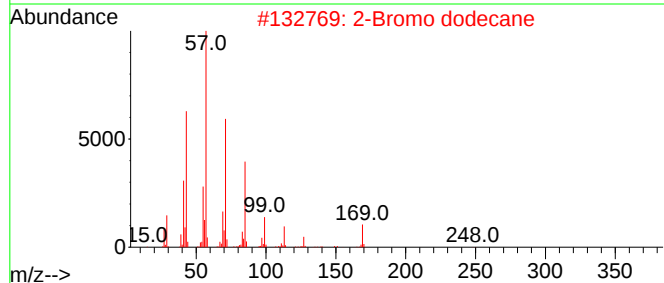
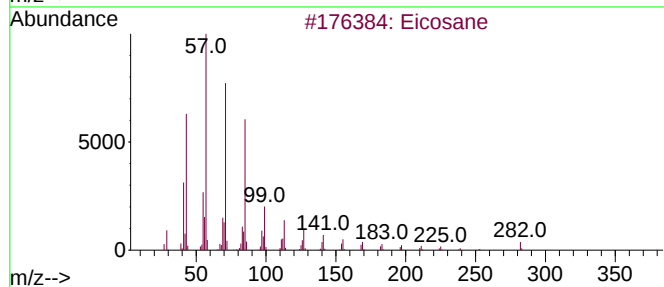
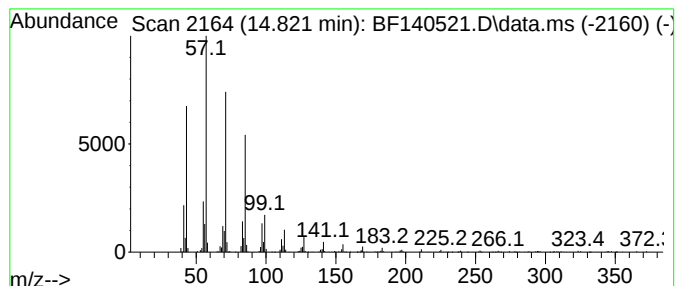
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 14 2-Bromo dodecane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD		R.T.	
14.822	14.73 ng	342321	Perylene-d12		15.545	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Eicosane		282	C20H42	000112-95-8	94
2	2-Bromo dodecane		248	C12H25Br	013187-99-0	93
3	Heneicosane		296	C21H44	000629-94-7	91
4	Dotriacontane, 1-iodo-		576	C32H65I	1000406-32-4	91
5	Tetracosane, 1-iodo-		464	C24H49I	1000406-32-0	91



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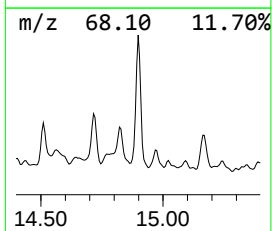
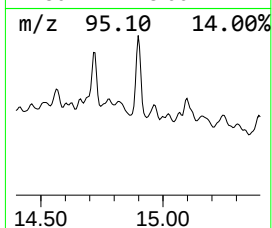
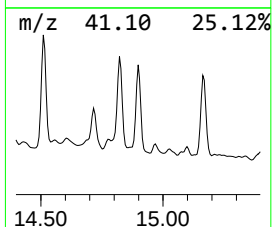
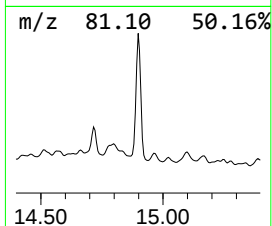
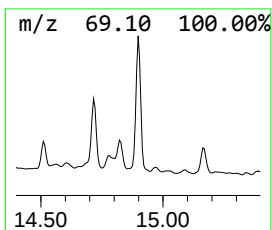
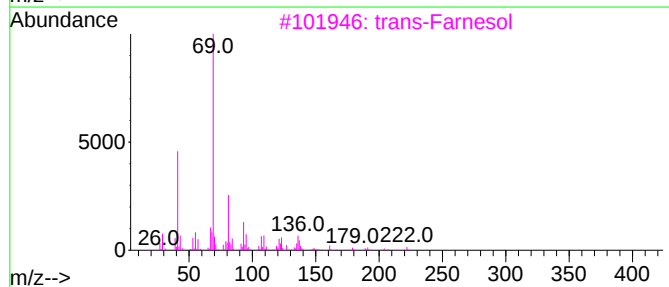
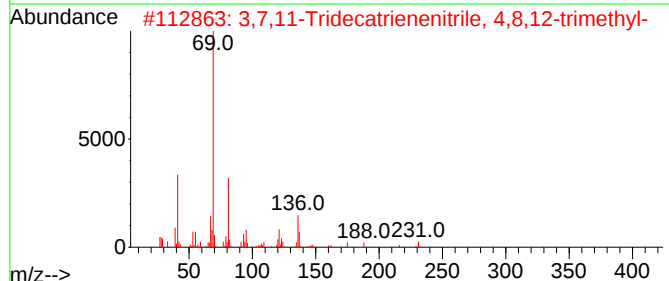
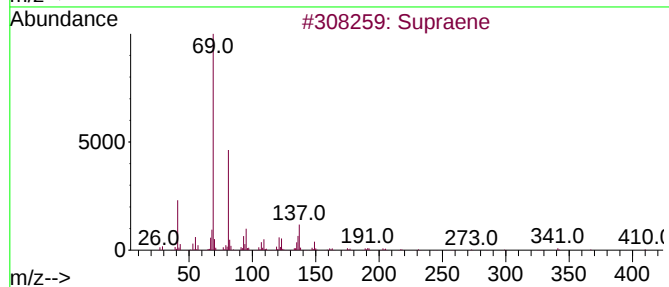
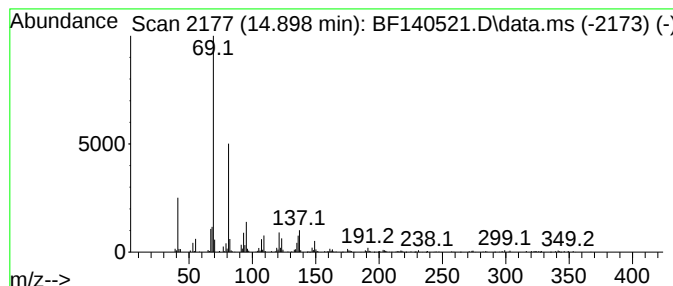
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 15 Supraene Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.898	8.94 ng	207831	Perylene-d12	15.545	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Supraene	410	C30H50	007683-64-9	87
2	3,7,11-Tridecatrienenitrile, 4,8...	231	C16H25N	006006-01-5	78
3	trans-Farnesol	222	C15H26O	000106-28-5	78
4	1,2-Epoxy-3,7,11-trimethyl-(6E,1...	238	C15H26O2	1000432-46-2	72
5	Farnesol (E), methyl ether	236	C16H28O	1000352-67-3	72



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF112024\
Data File : BF140521.D
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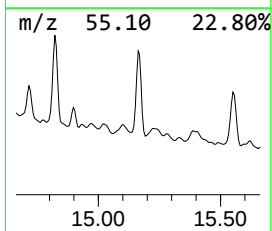
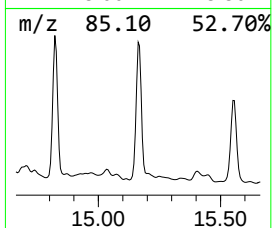
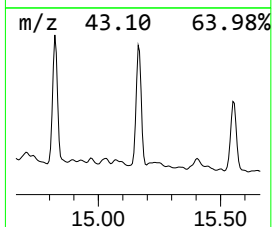
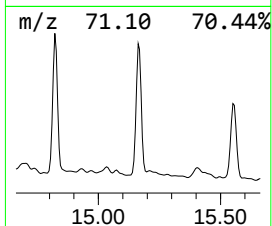
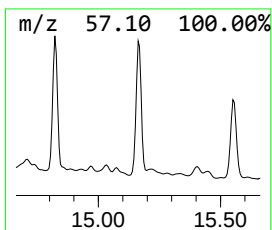
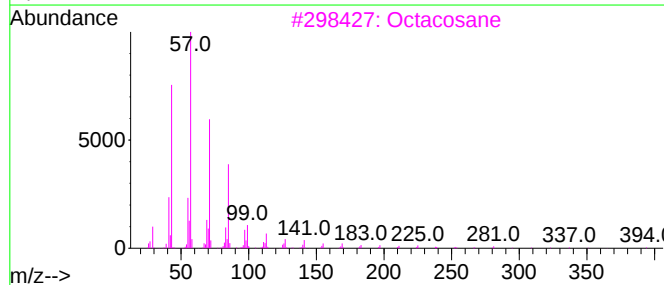
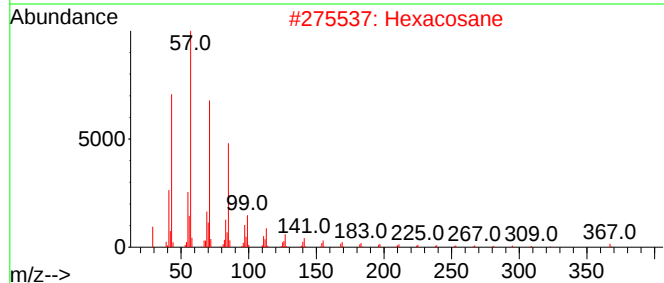
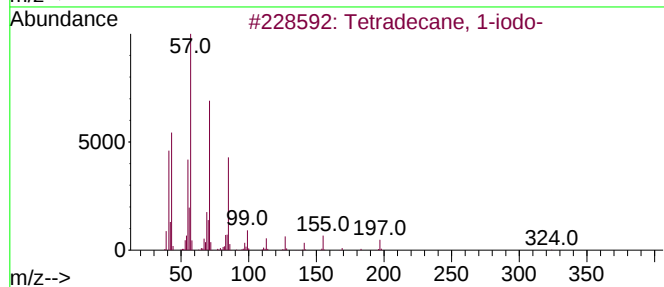
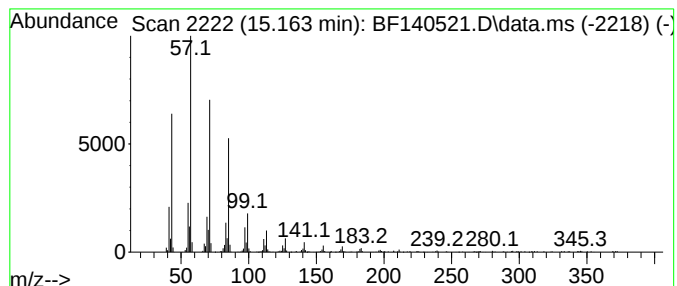
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 16 Tetradecane, 1-iodo- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.163	14.62 ng	339787	Perylene-d12	15.545

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetradecane, 1-iodo-	324	C14H29I	019218-94-1	93
2			Hexacosane	366	C26H54	000630-01-3	91
3			Octacosane	394	C28H58	000630-02-4	91
4			Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
5			Heptacosane	380	C27H56	000593-49-7	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF112024\
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Sample : P4860-02
Misc :
ALS Vial : 22 Sample Multiplier: 1

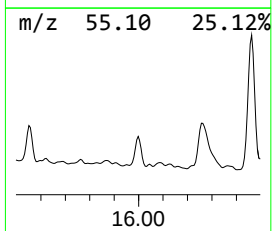
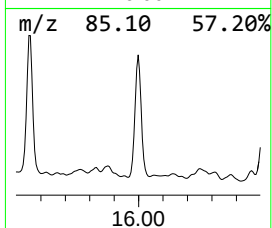
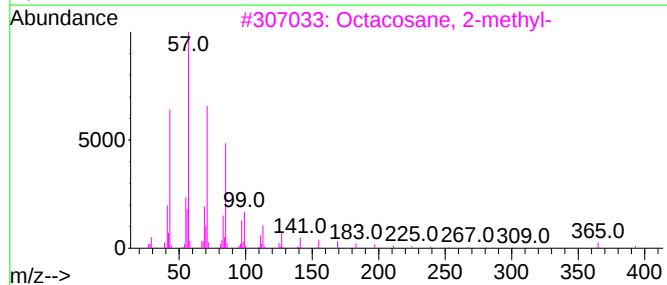
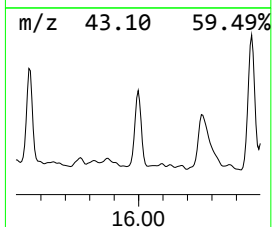
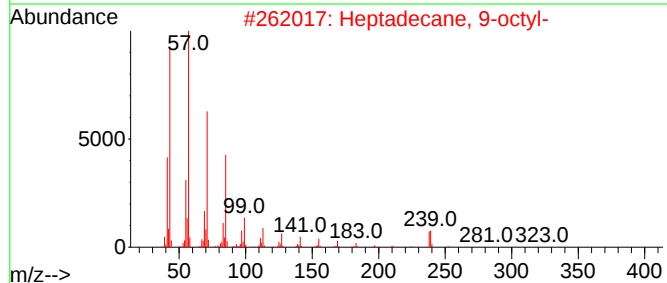
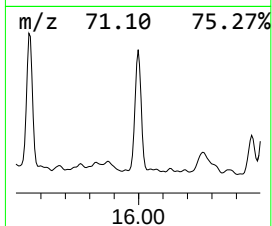
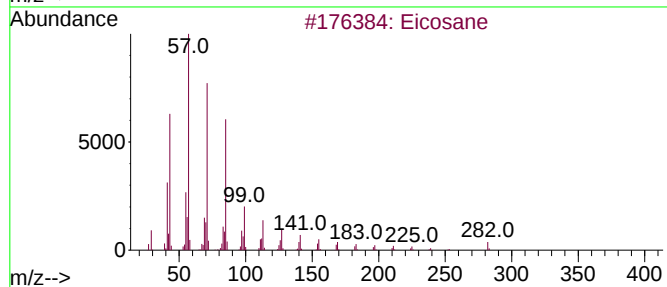
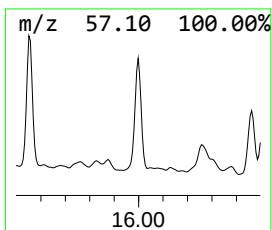
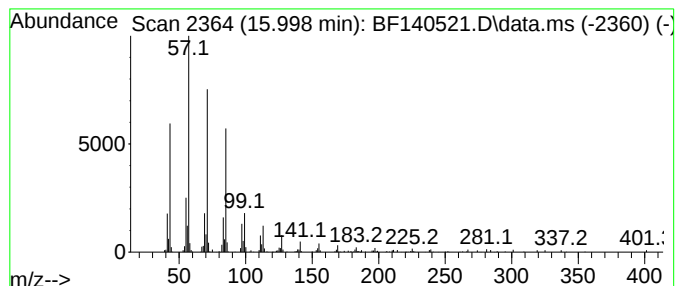
Instrument :
BNA_F
ClientSampleId :
PH2-BOT-001

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF111324.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 17 Heptadecane, 9-octyl- Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD		R.T.	
15.998	8.06 ng	187328	Perylene-d12		15.545	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Eicosane		282	C20H42	000112-95-8	94
2	Heptadecane, 9-octyl-		352	C25H52	007225-64-1	91
3	Octacosane, 2-methyl-		408	C29H60	001560-98-1	91
4	Heneicosane		296	C21H44	000629-94-7	91
5	Dotriacontane, 1-iodo-		576	C32H65I	1000406-32-4	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF112024\
Data File : BF140521.D
Acq On : 21 Nov 2024 00:51
Operator : RC/JU
Sample : P4860-02
Misc :
ALS Vial : 22 Sample Multiplier: 1

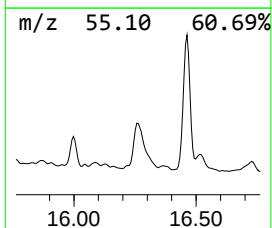
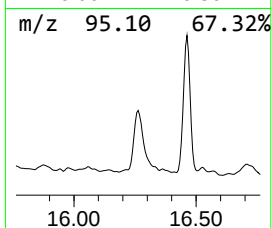
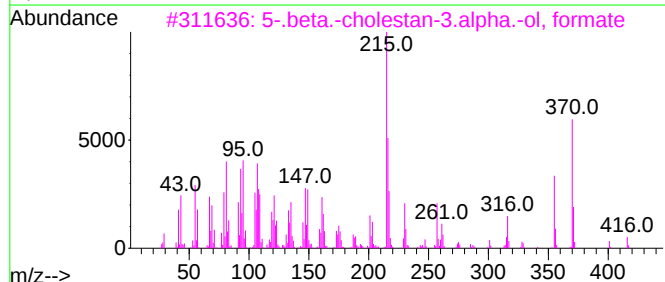
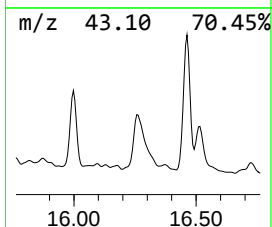
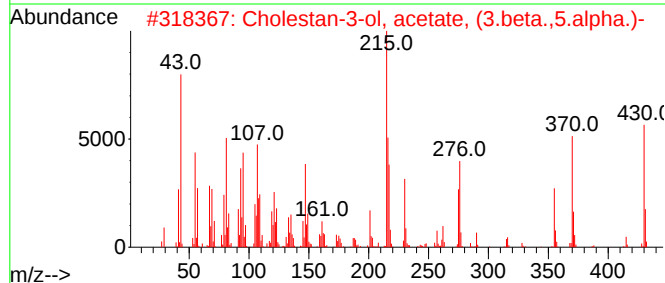
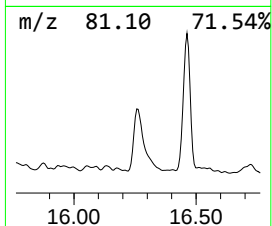
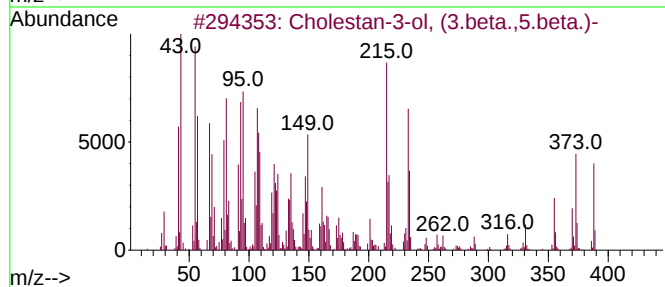
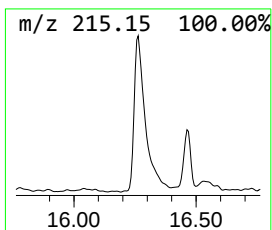
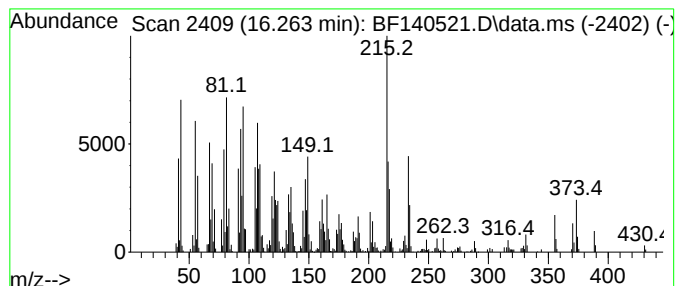
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ClientSampleId :
PH2-BOT-001

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF111324.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 18 Cholestan-3-ol, (3.beta.,5.... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.	
16.263	40.73 ng	946693	Perylene-d12	15.545	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cholestan-3-ol, (3.beta.,5.beta.)-	388	C27H48O	000360-68-9	97
2	Cholestan-3-ol, acetate, (3.beta...	430	C29H50O2	001255-88-5	86
3	5-.beta.-cholestan-3.alpha.-ol, ...	416	C28H48O2	1010368-37-5	64
4	5.beta.-Cholestan-3.alpha.-ol, 2...	458	C31H54O2	1000514-95-7	62
5	Cholestanol	388	C27H48O	000080-97-7	55



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF112024\
Data File : BF140521.D
Acq On : 21 Nov 2024 00:51
Operator : RC/JU
Sample : P4860-02
Misc :
ALS Vial : 22 Sample Multiplier: 1

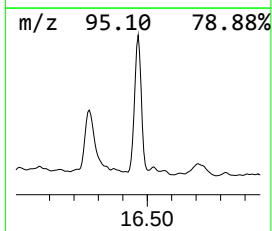
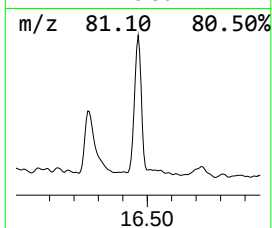
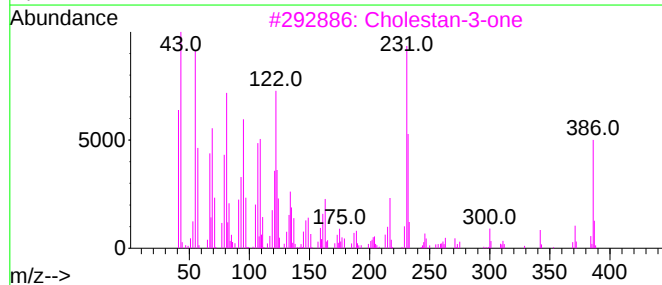
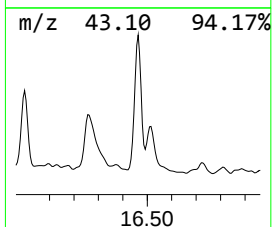
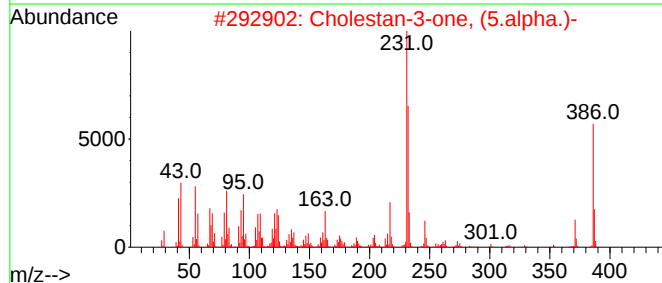
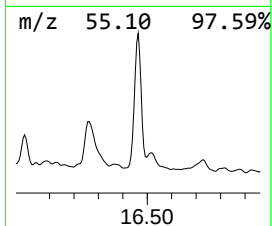
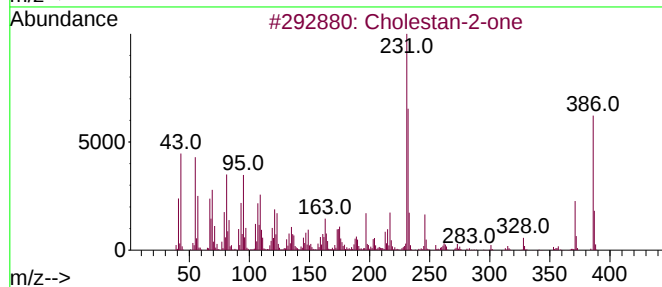
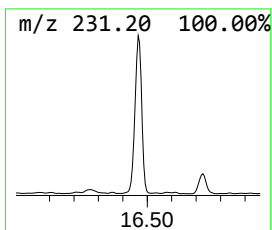
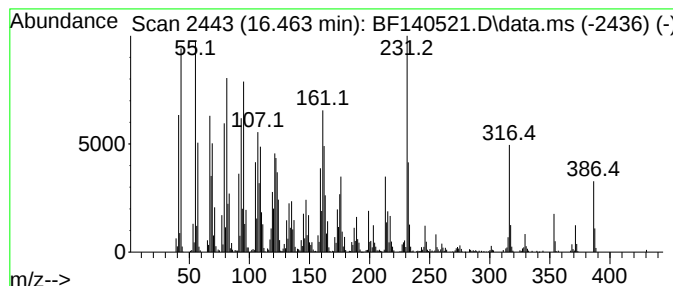
Instrument :
BNA_F
ClientSampleId :
PH2-BOT-001

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF111324.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 19 Cholestan-2-one Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.	
16.462	55.79 ng	1296900	Perylene-d12	15.545	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cholestan-2-one	386	C27H46O	1010210-43-4	95
2	Cholestan-3-one, (5.alpha.)-	386	C27H46O	000566-88-1	59
3	Cholestan-3-one	386	C27H46O	015600-08-5	49
4	Cholestan-3-one, (5.beta.)-	386	C27H46O	000601-53-6	49
5	Cholestane, 4,5-epoxy-, (4.alpha...	386	C27H46O	006079-19-2	46



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF112024\
Data File : BF140521.D
Acq On : 21 Nov 2024 00:51
Operator : RC/JU
Sample : P4860-02
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PH2-BOT-001

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF111324.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
Butane, 2-metho...	2.140	50.6	ng	986369	1	6.875	389528	20.0
n-Hexadecanoic ...	11.922	16.2	ng	414949	4	11.398	512200	20.0
4b,8-Dimethyl-2...	12.339	6.6	ng	168919	4	11.398	512200	20.0
10,18-Bisnorabi...	12.651	23.7	ng	607191	4	11.398	512200	20.0
Eicosane	12.851	5.6	ng	105189	5	14.045	373381	20.0
Retene	13.122	5.5	ng	103639	5	14.045	373381	20.0
Heneicosane	13.210	8.4	ng	156951	5	14.045	373381	20.0
Docosane, 1-iodo-	13.551	13.3	ng	249137	5	14.045	373381	20.0
Cyclohexane, 1,...	13.845	19.6	ng	366847	5	14.045	373381	20.0
Nonadecane	13.880	23.8	ng	444244	5	14.045	373381	20.0
Methadone N-oxide	14.175	12.0	ng	223505	5	14.045	373381	20.0
Tetracosane, 1-...	14.204	29.0	ng	542172	5	14.045	373381	20.0
Heptacosane	14.510	20.9	ng	390941	5	14.045	373381	20.0
2-Bromo dodecane	14.822	14.7	ng	342321	6	15.545	464920	20.0
Supraene	14.898	8.9	ng	207831	6	15.545	464920	20.0
Tetradecane, 1-...	15.163	14.6	ng	339787	6	15.545	464920	20.0
Heptadecane, 9-...	15.998	8.1	ng	187328	6	15.545	464920	20.0
Cholestan-3-ol,...	16.263	40.7	ng	946693	6	15.545	464920	20.0
Cholestan-2-one	16.462	55.8	ng	1296900	6	15.545	464920	20.0
17-(1,5-Dimethy...	17.674	13.3	ng	309715	6	15.545	464920	20.0