LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082224\
Data File : BF139122.D
Acq On : 22 Aug 2024 14:50
Operator : RC/JU
Sample : P3641-08
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
S-910-K1-0.5-1.0-081524-FD

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: BF139122.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.187	7	16	23	rBV	583889	883054	50.28%	3.335%
2	5.104	504	512	518	rBV	83912	116974	6.66%	0.442%
3	5.510	575	581	586	rBV	718684	901515	51.33%	3.405%
4	6.446	734	740	746	rBV2	42404	54388	3.10%	0.205%
5	6.516	746	752	756	rBV	673028	874475	49.79%	3.303%
6	6.898	812	817	822	rBV	416520	510177	29.05%	1.927%
7	7.051	836	843	848	rBV	72899	90706	5.16%	0.343%
8	7.298	880	885	889	rBV	18854	22912	1.30%	0.087%
9	7.451	903	911	916	rBV	445120	567490	32.31%	2.143%
10	7.863	974	981	989	rBV	31227	55787	3.18%	0.211%
11	8.181	1029	1035	1042	rBV	480631	624227	35.54%	2.358%
12	8.487	1083	1087	1096	rBV	29139	38245	2.18%	0.144%
13	8.892	1152	1156	1160	rBV	40144	50854	2.90%	0.192%
14	8.934	1160	1163	1169	rVB	14334	18786	1.07%	0.071%
15	9.251	1212	1217	1222	rBV	765447	906908	51.64%	3.425%
16	9.792	1305	1309	1314	rBV	42368	50924	2.90%	0.192%
17	9.934	1326	1333	1337	rBV	457182	589162	33.55%	2.225%
18	9.963	1337	1338	1342	rVB	32148	23797	1.36%	0.090%
19	10.028	1344	1349	1352	rBV3	15208	25412	1.45%	0.096%
20	10.134	1363	1367	1371	rBV	21000	26628	1.52%	0.101%
21	10.475	1422	1425	1430	rVB	23943	30975	1.76%	0.117%
22	10.716	1459	1466	1471	rBV	367315	458935	26.13%	1.733%
23	10.839	1483	1487	1494	rVB3	34097	44911	2.56%	0.170%
24	11.028	1512	1519	1522	rBV6	9414	19864	1.13%	0.075%
25	11.175	1536	1544	1547	rBV5	13426	30683	1.75%	0.116%
26	11.216	1547	1551	1556	rVB2	29407	41245	2.35%	0.156%
27	11.281	1556	1562	1565	rBV5	17609	36391	2.07%	0.137%
28	11.310	1565	1567	1571	rVB	23726	27999	1.59%	0.106%
29	11.416	1580	1585	1587	rVV	394093	519051	29.56%	1.960%
30	11.439	1587	1589	1594	rVV	452178	531817	30.28%	2.009%
31	11.492	1594	1598	1601	rVV	86010	110704	6.30%	0.418%
32	11.528	1601	1604	1610	rVB5	19626	28175	1.60%	0.106%
33	11.645	1618	1624	1633	rBV2	55642	106822	6.08%	0.403%
34	11.822	1646	1654	1656	rBV7	12117	28830	1.64%	0.109%
35	11.916	1665	1670	1671	rBV2	74885	99379	5.66%	0.375%
36	11.945	1671	1675	1679	rVV	233617	323359	18.41%	1.221%

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082224\
Data File : BF139122.D
Acq On : 22 Aug 2024 14:50
Operator : RC/JU
Sample : P3641-08
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
S-910-K1-0.5-1.0-081524-FD

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

37	11.992	1679	1683	1685	rVV2	26787	38525	2.19%	0.145%
38	12.028	1685	1689	1698	rVB	101381	187263	10.66%	0.707%
39	12.122	1698	1705	1708	rBV3	20975	44971	2.56%	0.170%
40	12.233	1717	1724	1730	rVB2	104494	192312	10.95%	0.726%
41	12.363	1740	1746	1749	rBV2	19646	34860	1.98%	0.132%
42	12.469	1759	1764	1767	rBV	62662	88405	5.03%	0.334%
43	12.504	1767	1770	1775	rVV3	27622	45582	2.60%	0.172%
44	12.551	1775	1778	1784	rVB2	62938	90028	5.13%	0.340%
45	12.633	1786	1792	1805	rBV	1252836	1756197	100.00%	6.633%
46	12.727	1805	1808	1811	rBV3	45672	57430	3.27%	0.217%
47	12.780	1815	1817	1823	rVB3	32670	42033	2.39%	0.159%
48	12.863	1823	1831	1837	rBV	1001603	1618501	92.16%	6.113%
49	13.004	1843	1855	1861	rVB	599502	881733	50.21%	3.330%
50	13.075	1861	1867	1875	rBV3	100333	231153	13.16%	0.873%
51	13.186	1878	1886	1889	rBV2	126984	252849	14.40%	0.955%
52	13.251	1893	1897	1900	rVV2	79460	96290	5.48%	0.364%
53	13.286	1900	1903	1907	rVV2	97066	129958	7.40%	0.491%
54	13.351	1911	1914	1916	rBV	17615	22056	1.26%	0.083%
55	13.380	1916	1919	1922	rBV	44624	52883	3.01%	0.200%
56	13.416	1922	1925	1928	rBV2	35128	44430	2.53%	0.168%
57	13.586	1947	1954	1956	rBV7	42414	99885	5.69%	0.377%
58	13.692	1968	1972	1986	rVB	155659	344876	19.64%	1.302%
59	13.804	1986	1991	1994	rBV2	136595	214897	12.24%	0.812%
60	13.833	1994	1996	1998	rBV	44845	47516	2.71%	0.179%
61	13.904	2003	2008	2014	rVB3	261176	405075	23.07%	1.530%
62	14.051	2027	2033	2036	rBV2	842804	1446233	82.35%	5.462%
63	14.080	2036	2038	2044	rVB	549097	720626	41.03%	2.722%
64	14.163	2049	2052	2055	rVB	62482	75100	4.28%	0.284%
65	14.274	2068	2071	2075	rVB2	38116	50598	2.88%	0.191%
66	14.439	2096	2099	2102	rBV	78109	90133	5.13%	0.340%
67	14.474	2102	2105	2109	rVB3	87082	111576	6.35%	0.421%
68	14.539	2111	2116	2123	rBV3	425853	691234	39.36%	2.611%
69	14.751	2148	2152	2162	rVB6	90113	186715	10.63%	0.705%
70	14.839	2163	2167	2177	rBV8	46378	125143	7.13%	0.473%
71	14.921	2178	2181	2188	rVB3	45145	81713	4.65%	0.309%
72	14.998	2189	2194	2199	rBV2	222409	333789	19.01%	1.261%
73	15.104	2206	2212	2222	rVV	564827	1286622	73.26%	4.859%
74	15.216	2223	2231	2238	rVB3	445936	1133937	64.57%	4.283%
75	15.410	2259	2264	2269	rVB	269783	408208	23.24%	1.542%
76	15.468	2269	2274	2280	rBV	327299	522485	29.75%	1.973%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082224\
Data File : BF139122.D
Acq On : 22 Aug 2024 14:50
Operator : RC/JU
Sample : P3641-08
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
S-910-K1-0.5-1.0-081524-FD

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

77	15.533	2281	2285	2289	rBV	216562	330260	18.81%	1.247%
78	15.792	2325	2329	2337	rVB2	140775	232962	13.27%	0.880%
79	16.039	2365	2371	2375	rBV	308524	551027	31.38%	2.081%
80	16.086	2375	2379	2387	rVB2	154795	308995	17.59%	1.167%
81	16.857	2504	2510	2518	rVB3	134488	286441	16.31%	1.082%
82	17.015	2531	2537	2549	rBV2	169134	438318	24.96%	1.655%
83	17.174	2559	2564	2568	rBV	47477	114518	6.52%	0.433%
84	17.257	2575	2578	2590	rVB3	91267	214171	12.20%	0.809%
85	17.462	2608	2613	2634	rVB	129284	324888	18.50%	1.227%
86	17.639	2637	2643	2650	rBV3	123157	301648	17.18%	1.139%
87	17.986	2696	2702	2710	rBV3	87226	219532	12.50%	0.829%

Sum of corrected areas: 26478141

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082224\
Data File : BF139122.D
Acq On : 22 Aug 2024 14:50
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Misc :
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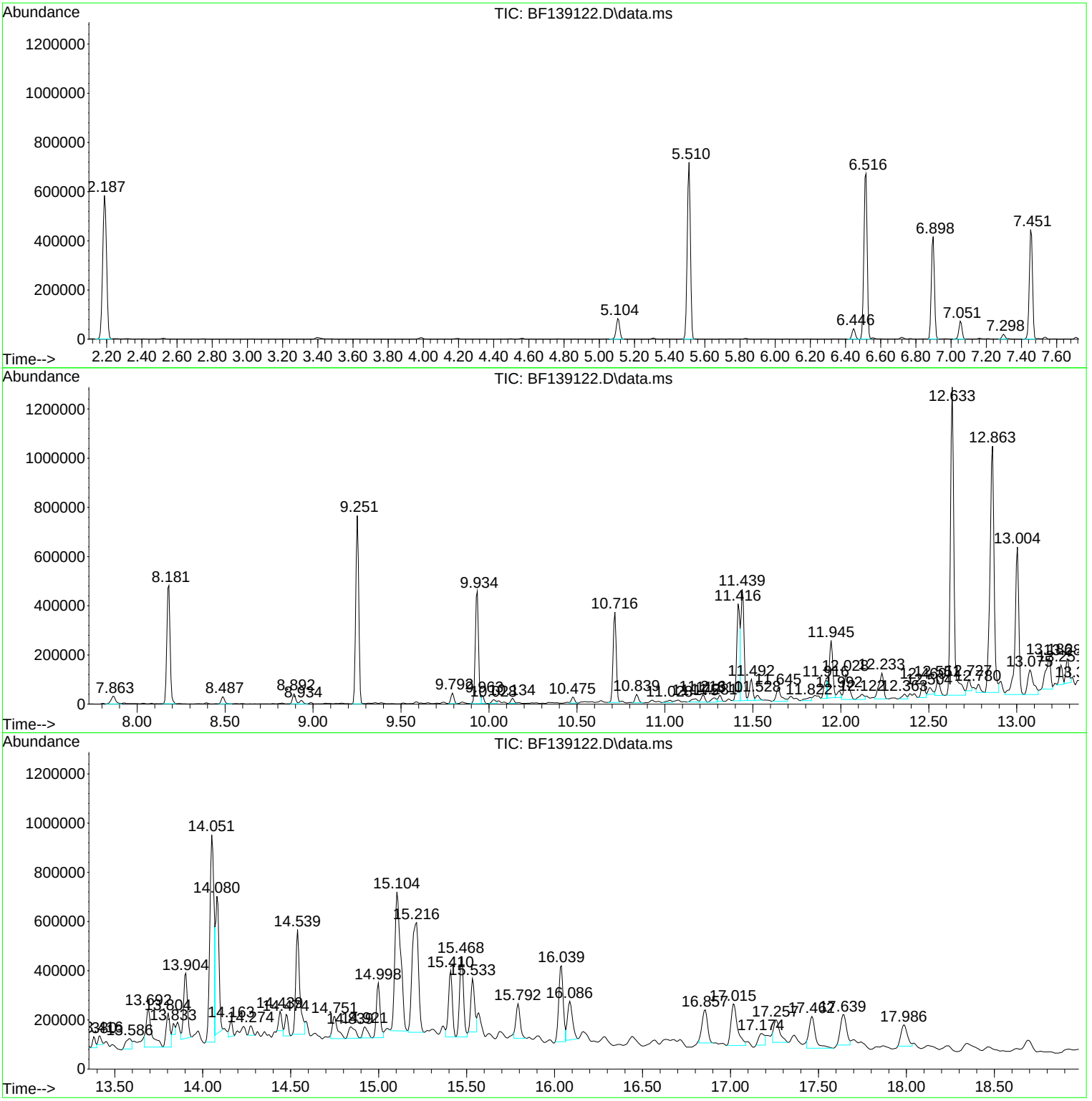
Instrument :
BNA_F
ClientSampleId :
S-910-K1-0.5-1.0-081524-FD

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\
Data File : BF139122.D
Acq On : 22 Aug 2024 14:50
Operator : RC/JU
Sample : P3641-08
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
S-910-K1-0.5-1.0-081524-FD

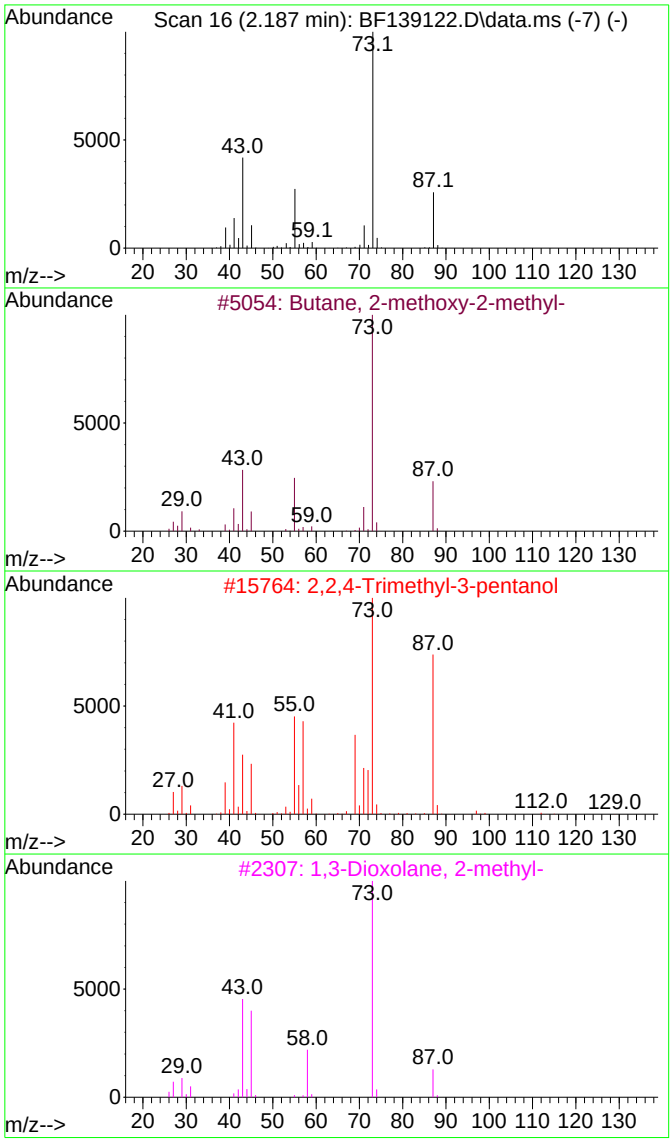
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF082024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

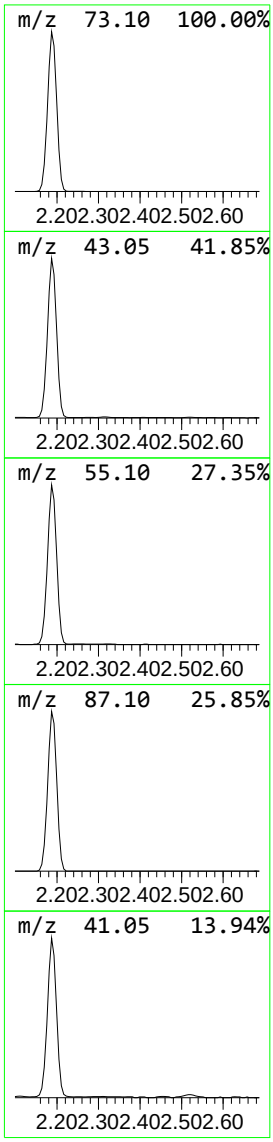
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.187	34.62 ng	883054	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	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
4	Octanal, 7-methoxy-3,7-dimethyl-	186	C11H22O2	003613-30-7	17
5	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082224\
Data File : BF139122.D
Acq On : 22 Aug 2024 14:50
Operator : RC/JU
Sample : P3641-08
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
S-910-K1-0.5-1.0-081524-FD

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

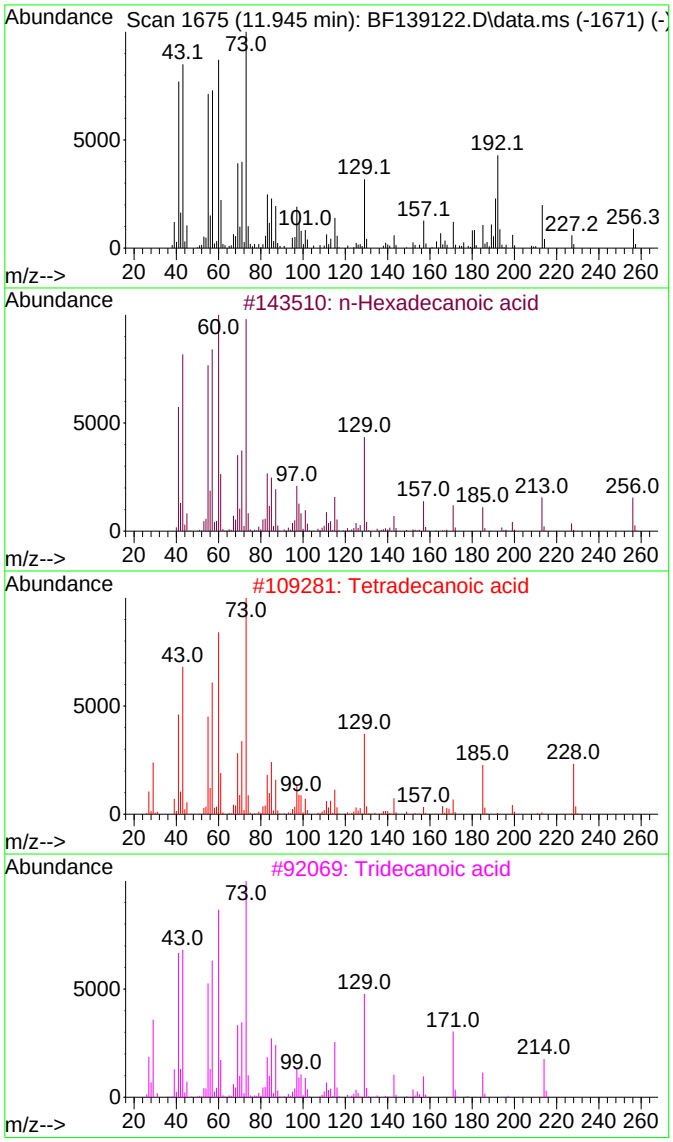
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

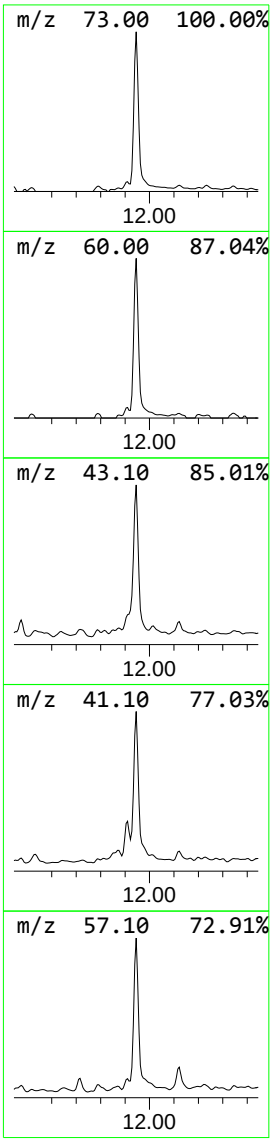
****

Peak Number 2 n-Hexadecanoic acid Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.945	12.46 ng	323359	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	93
3	Tridecanoic acid	214	C13H26O2	000638-53-9	91
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	64
5	Nonanoic acid	158	C9H18O2	000112-05-0	30





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082224\
Data File : BF139122.D
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Sample : P3641-08
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
S-910-K1-0.5-1.0-081524-FD

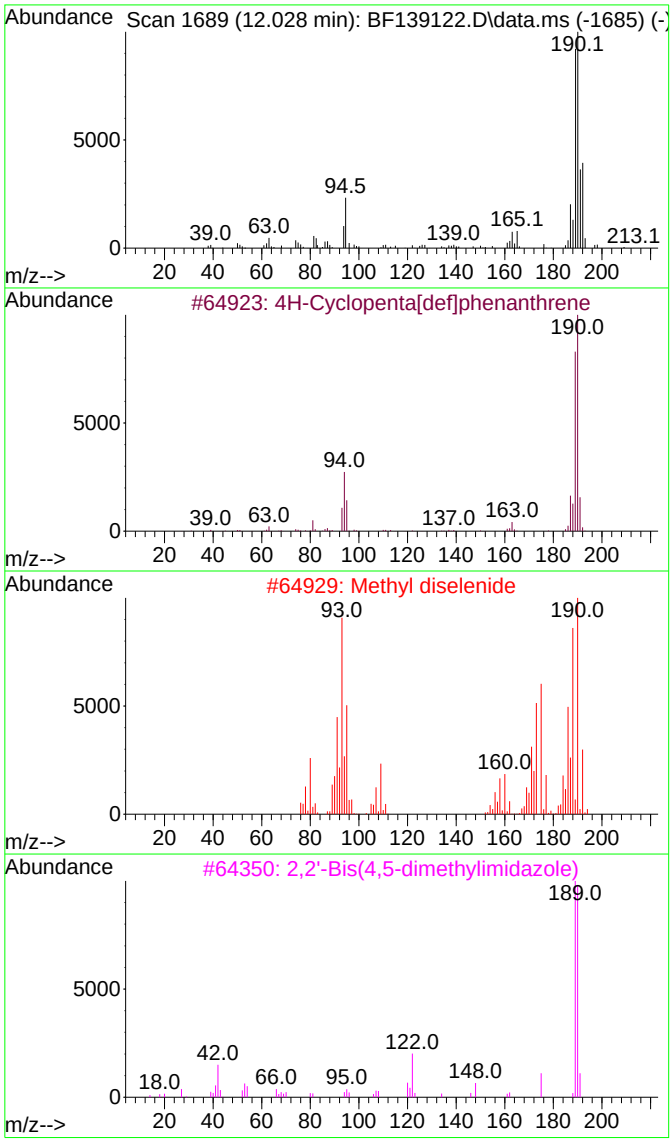
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF082024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

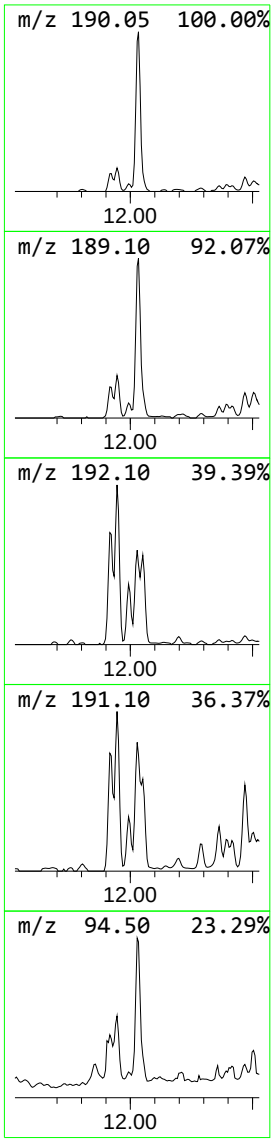
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 4H-Cyclopenta[def]phenanthrene Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.028	7.22 ng	187263	Phenanthrene-d10	11.416

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	81
2	Methyl diselenide	190	C2H6Se2	007101-31-7	43
3	2,2'-Bis(4,5-dimethylimidazole)	190	C10H14N4	069286-06-2	38
4	6H-Cyclobuta[jk]phenanthrene	190	C15H10	083469-43-6	28
5	1,4-Naphthalenedione, 2,5-dihydr...	190	C10H6O4	004923-55-1	27





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082224\
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Sample : P3641-08
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
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S-910-K1-0.5-1.0-081524-FD

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

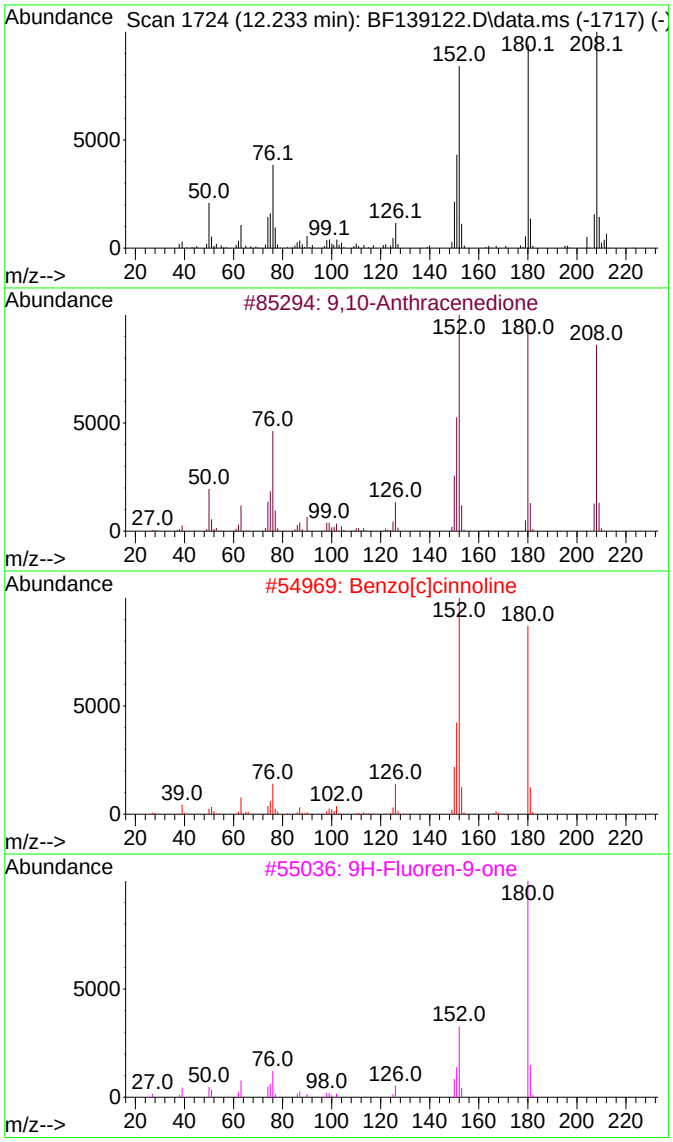
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

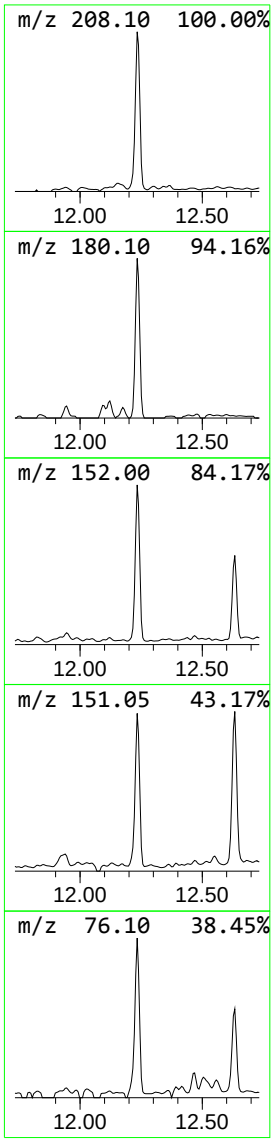
****

Peak Number 4 9,10-Anthracenedione Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.233	7.41 ng	192312	Phenanthrene-d10	11.416

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9,10-Anthracenedione	208	C14H8O2	000084-65-1	99
2	Benzo[c]cinnoline	180	C12H8N2	000230-17-1	95
3	9H-Fluoren-9-one	180	C13H8O	000486-25-9	90
4	9,10-Phenanthrenedione	208	C14H8O2	000084-11-7	55
5	1H-Phenalen-1-one	180	C13H8O	000548-39-0	53





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082224\
Data File : BF139122.D
Acq On : 22 Aug 2024 14:50
Operator : RC/JU
Sample : P3641-08
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
S-910-K1-0.5-1.0-081524-FD

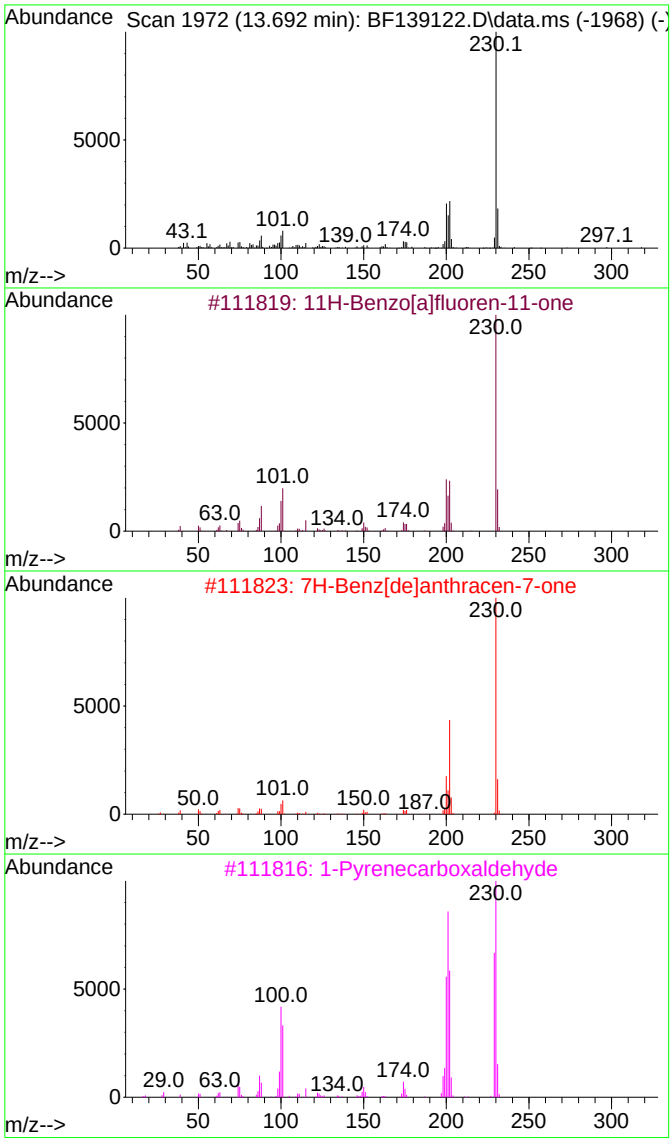
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF082024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

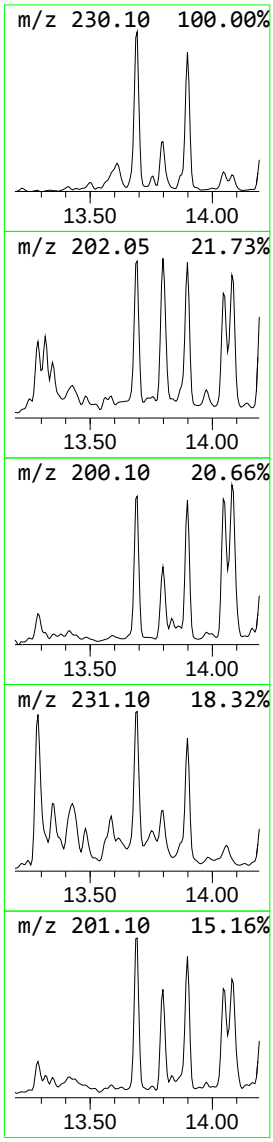
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 11H-Benzo[a]fluoren-11-one Concentration Rank 20

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.692	4.77 ng	344876	Chrysene-d12	14.057

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	11H-Benzo[a]fluoren-11-one	230	C17H10O	000479-79-8	94
2	7H-Benz[de]anthracen-7-one	230	C17H10O	000082-05-3	81
3	1-Pyrenecarboxaldehyde	230	C17H10O	003029-19-4	72
4	6H-Benz[de]anthracen-6-one	230	C17H10O	080252-14-8	64
5	.delta.(sup1),.alpha.-Acenaphthe...	230	C15H6N2O	014619-86-4	59





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082224\
Data File : BF139122.D
Acq On : 22 Aug 2024 14:50
Operator : RC/JU
Sample : P3641-08
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
S-910-K1-0.5-1.0-081524-FD

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

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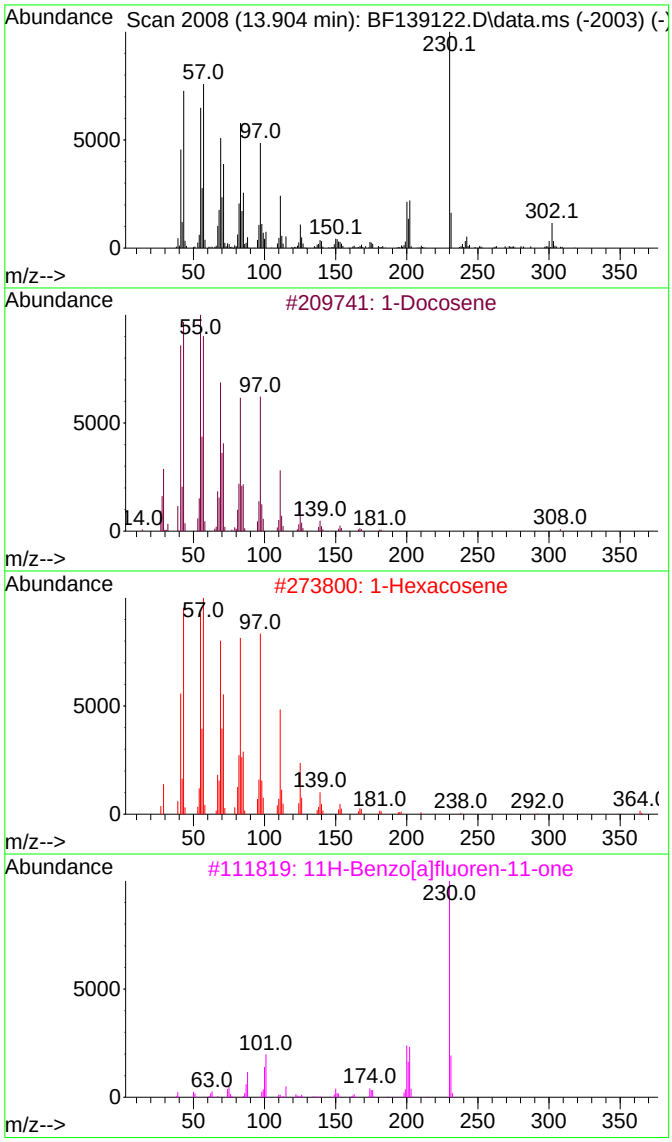
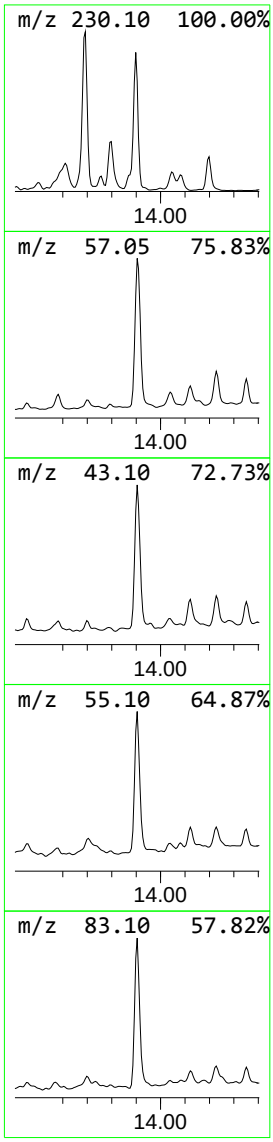
Peak Number 6 1-Docosene Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.904	5.60 ng	405075	Chrysene-d12	14.057

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Docosene	308	C22H44	001599-67-3	94
2	1-Hexacosene	364	C26H52	018835-33-1	64
3	11H-Benzo[a]fluoren-11-one	230	C17H10O	000479-79-8	56
4	Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	50
5	1-Heneicosyl formate	340	C22H44O2	077899-03-7	50





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Acq On : 22 Aug 2024 14:50
Operator : RC/JU
Sample : P3641-08
Misc :
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Instrument :
BNA_F
ClientSampleId :
S-910-K1-0.5-1.0-081524-FD

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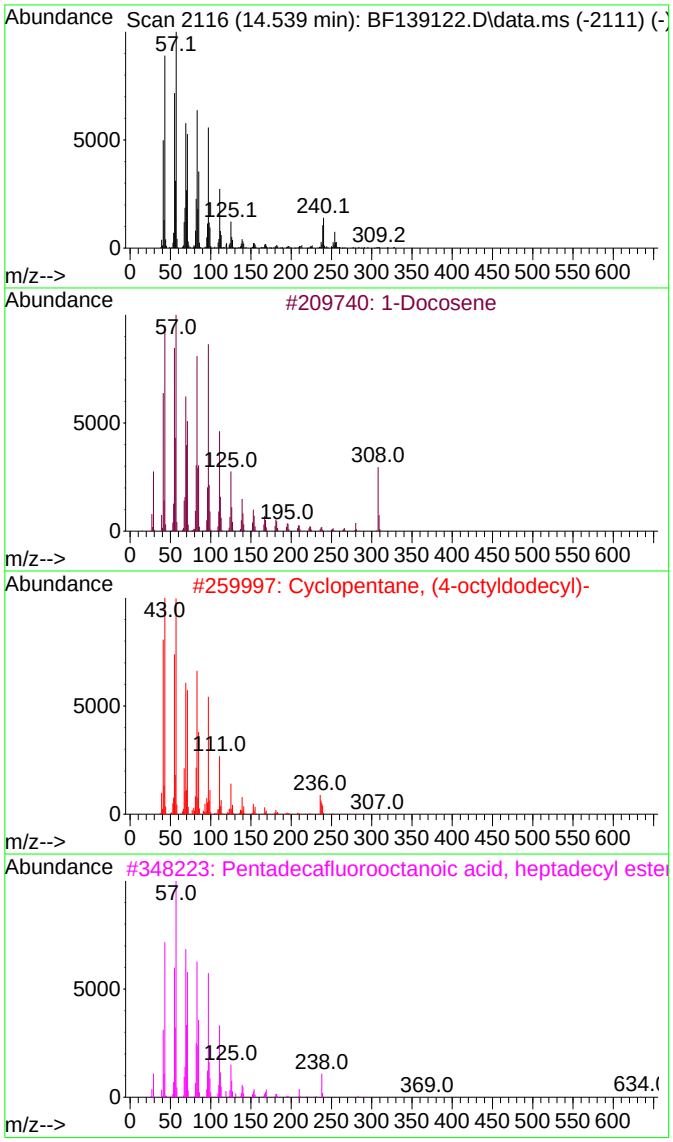
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

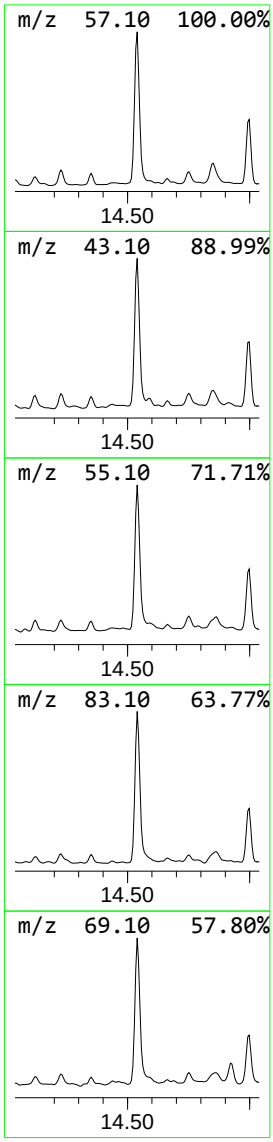
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Cyclopentane, (4-octyldodec... Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.539	9.56 ng	691234	Chrysene-d12	14.057

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Docosene	308	C22H44	001599-67-3	97
2	Cyclopentane, (4-octyldodecyl)-	350	C25H50	005638-09-5	93
3	Pentadecafluorooctanoic acid, he...	652	C25H35F15O2	1000406-04-7	91
4	Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	91
5	1-Heneicosanol	312	C21H44O	015594-90-8	91





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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

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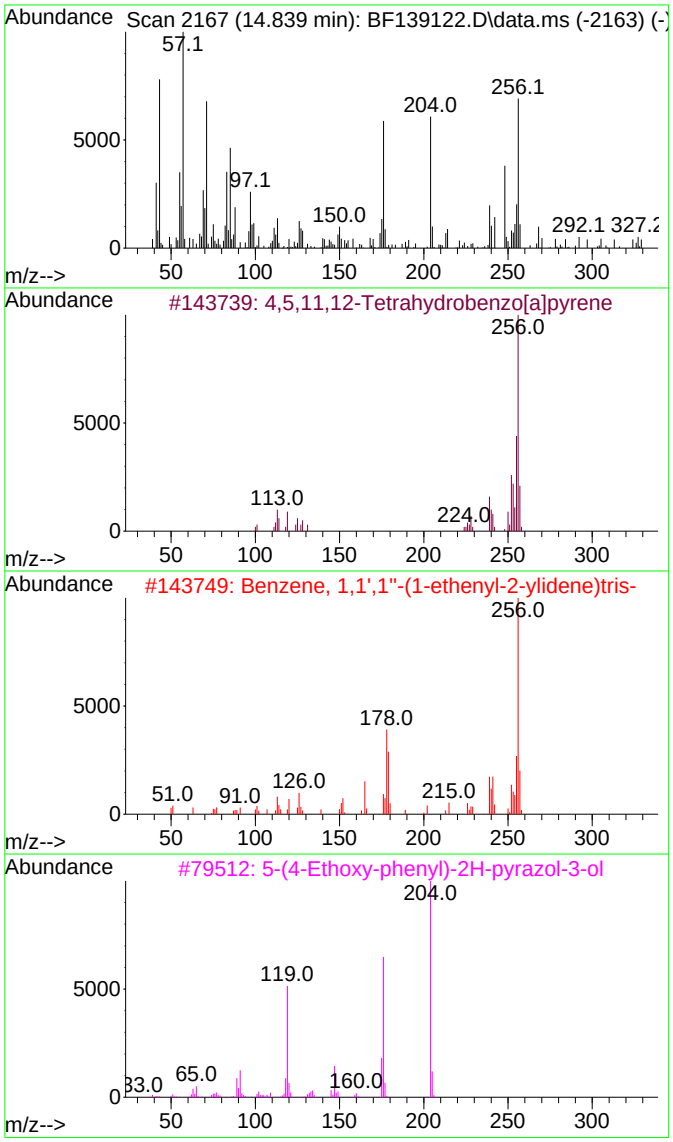
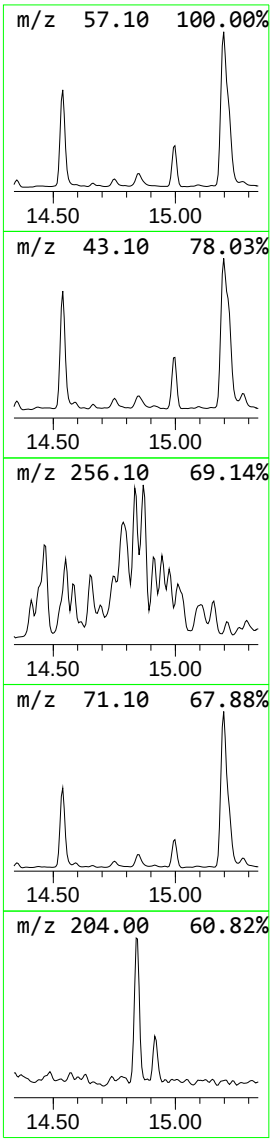
Peak Number 8 unknown14.839 Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.839	7.58 ng	125143	Perylene-d12	15.533

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4,5,11,12-Tetrahydrobenzo[a]pyrene	256	C20H16	109292-58-2	22
2	Benzene, 1,1',1''-(1-ethenyl-2-y...	256	C20H16	000058-72-0	20
3	5-(4-Ethoxy-phenyl)-2H-pyrazol-3-ol	204	C11H12N2O2	1000278-26-8	18
4	8,9,10,11-Tetrahydrobenzo[k]fluo...	256	C20H16	033942-81-3	14
5	6,6'-Biquinoline	256	C18H12N2	000612-79-3	11





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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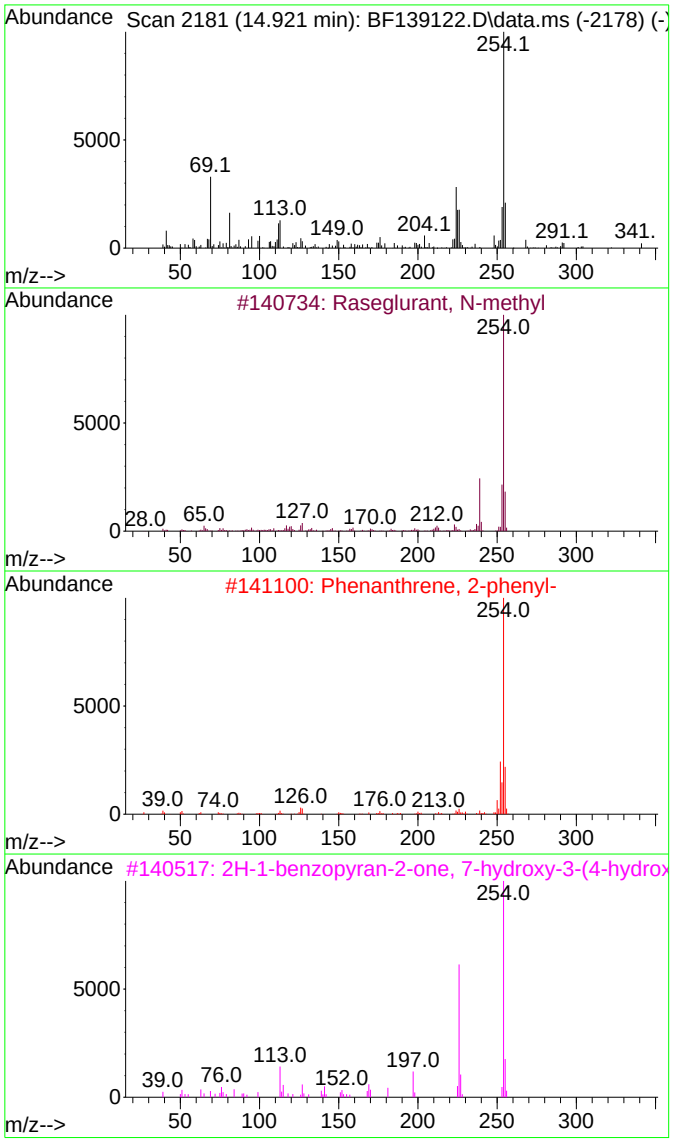
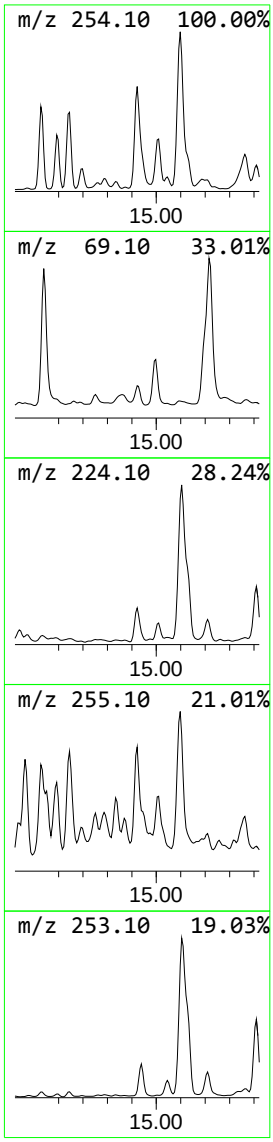
Peak Number 9 Raseglurant, N-methyl Concentration Rank 19

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.922	4.95 ng	81713	Perylene-d12	15.533

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Raseglurant, N-methyl	254	C16H15FN2	1000498-91-9	58
2	Phenanthrene, 2-phenyl-	254	C20H14	004325-77-3	58
3	2H-1-benzopyran-2-one, 7-hydroxy...	254	C15H10O4	1000401-42-6	47
4	1,1'-Binaphthalene	254	C20H14	000604-53-5	47
5	Benzo(e)pyrene, 9,10-dihydro-	254	C20H14	066788-01-0	47





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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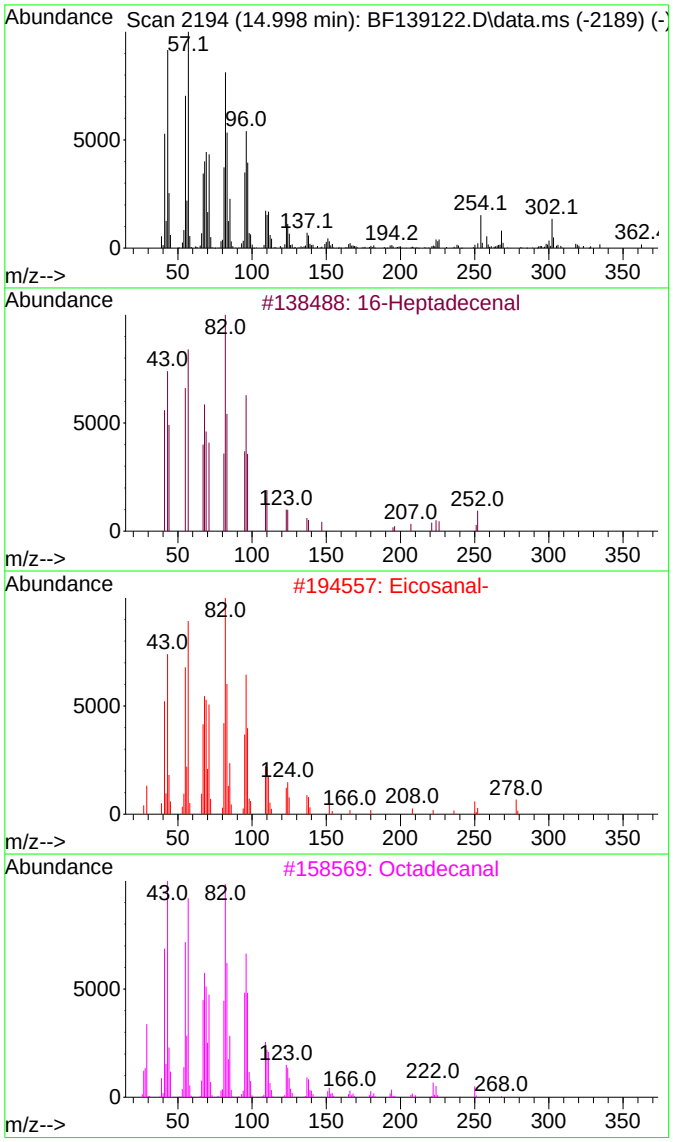
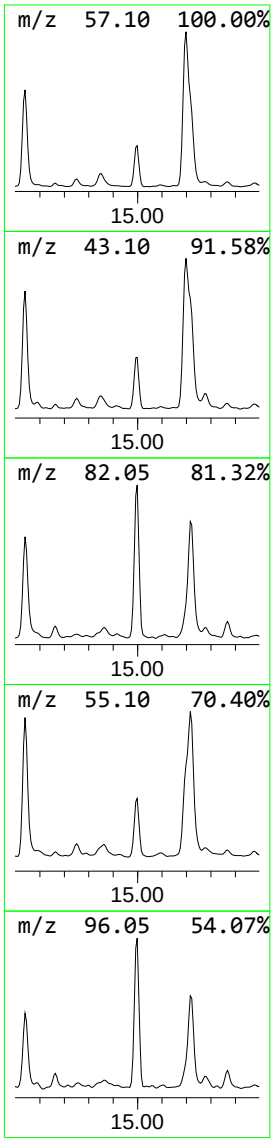
Peak Number 10 16-Heptadecenal Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.998	20.21 ng	333789	Perylene-d12	15.533

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	16-Heptadecenal	252	C17H32O	1010144-57-9	97
2	Eicosanal-	296	C20H40O	002400-66-0	94
3	Octadecanal	268	C18H36O	000638-66-4	94
4	Oxirane, heptadecyl-	282	C19H38O	067860-04-2	91
5	Oxirane, hexadecyl-	268	C18H36O	007390-81-0	91





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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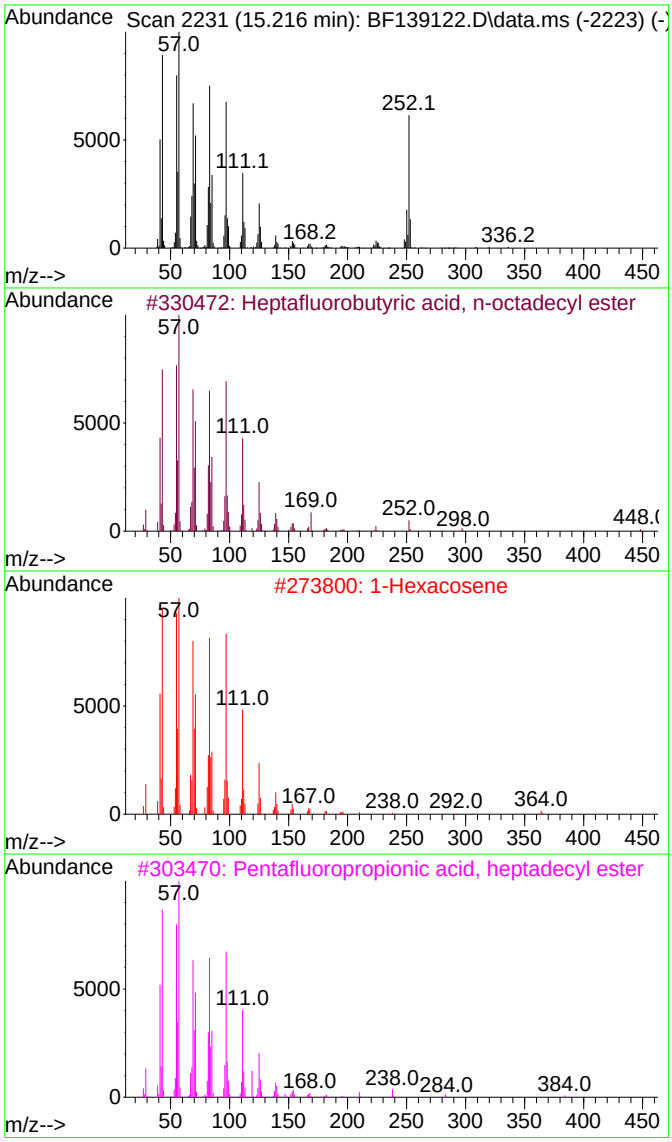
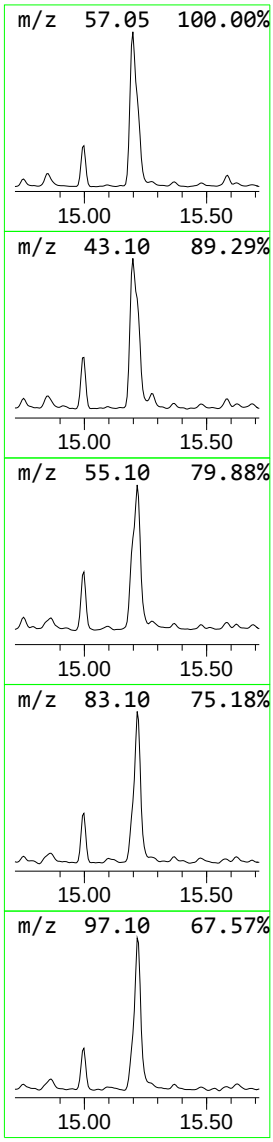
Peak Number 11 Heptafluorobutyric acid, n-... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.216	68.67 ng	1133940	Perylene-d12	15.533

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptafluorobutyric acid, n-octad...	466	C22H37F7O2	000400-57-7	90
2	1-Hexacosene	364	C26H52	018835-33-1	90
3	Pentafluoropropionic acid, hepta...	402	C20H35F5O2	959218-78-1	90
4	Heptafluorobutyric acid, hexadec...	438	C20H33F7O2	006385-15-5	90
5	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	90





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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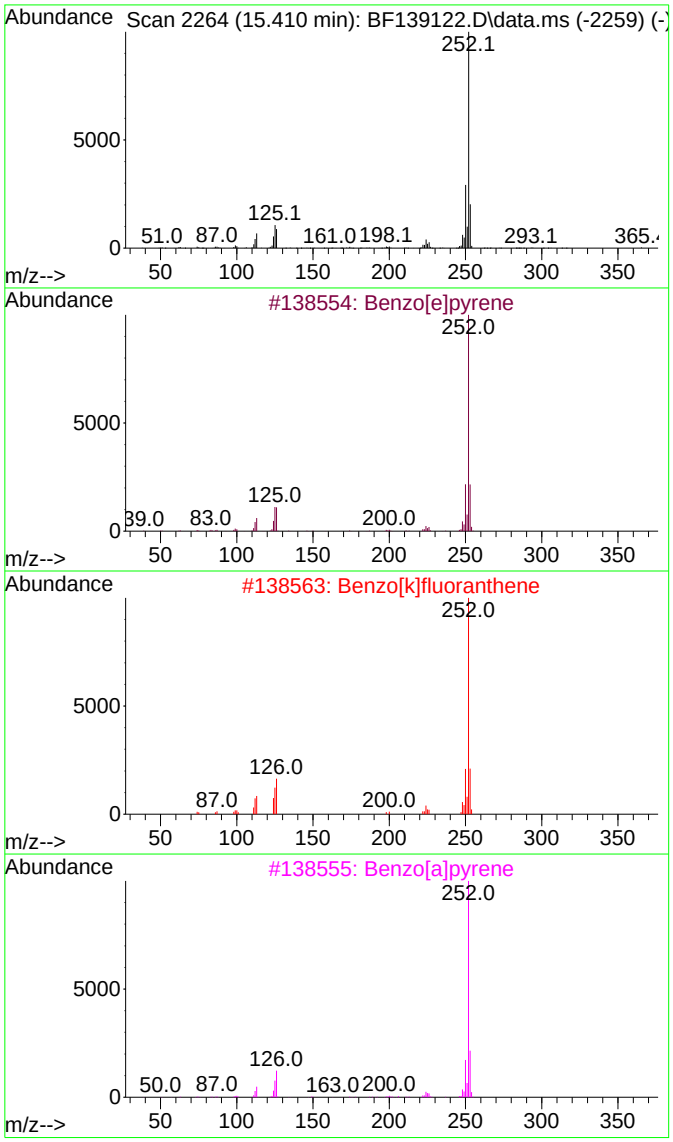
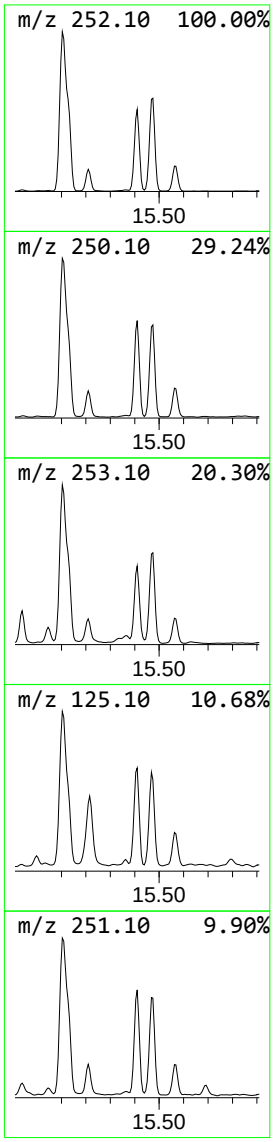
Peak Number 12 Benzo[e]pyrene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.410	24.72 ng	408208	Perylene-d12	15.533

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[e]pyrene	252	C20H12	000192-97-2	94
2	Benzo[k]fluoranthene	252	C20H12	000207-08-9	93
3	Benzo[a]pyrene	252	C20H12	000050-32-8	93
4	Benzo[b]fluoranthene	252	C20H12	000205-99-2	93
5	Perylene	252	C20H12	000198-55-0	90





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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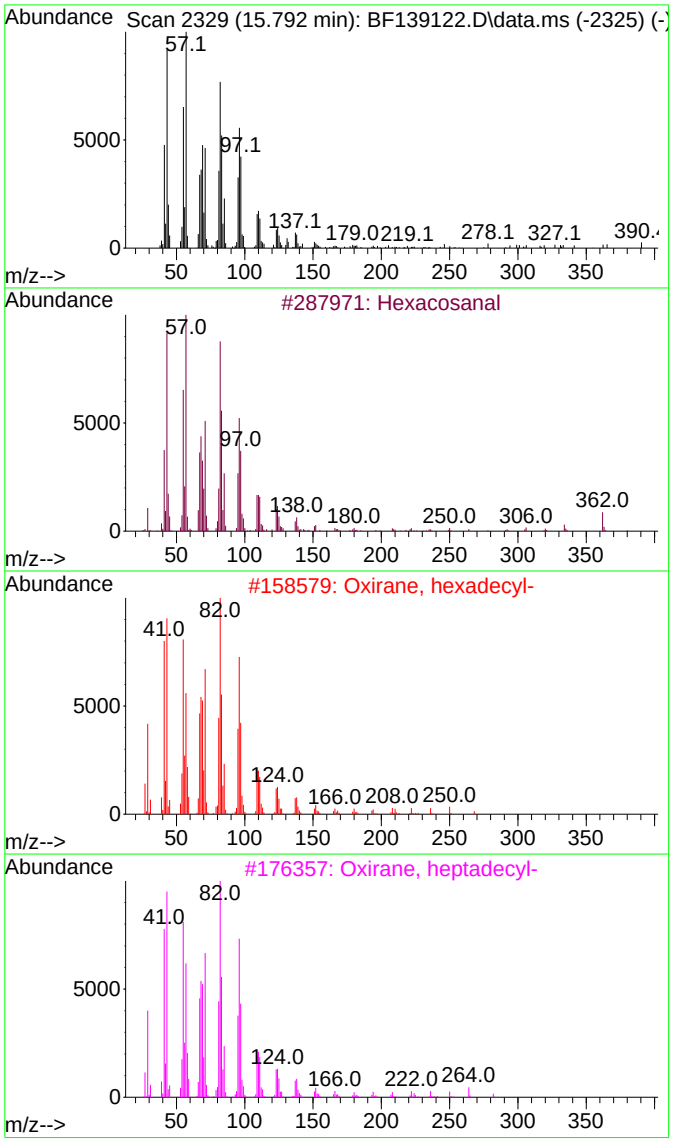
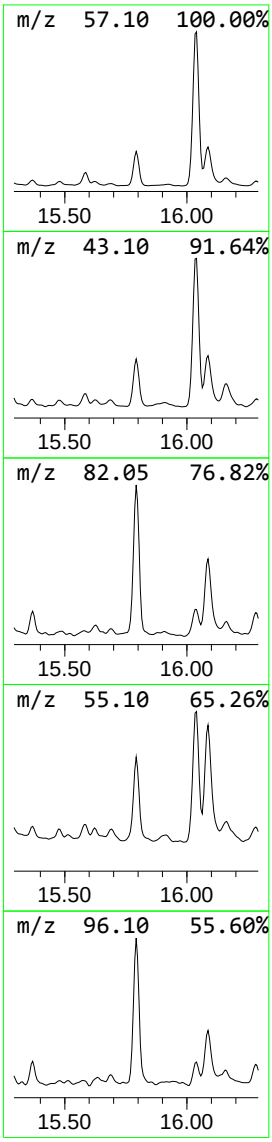
Peak Number 13 Hexacosanal Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.792	14.11 ng	232962	Perylene-d12	15.533

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosanal	380	C26H52O	026627-85-0	94
2	Oxirane, hexadecyl-	268	C18H36O	007390-81-0	94
3	Oxirane, heptadecyl-	282	C19H38O	067860-04-2	94
4	Octadecanal	268	C18H36O	000638-66-4	90
5	Docosanal	324	C22H44O	057402-36-5	90





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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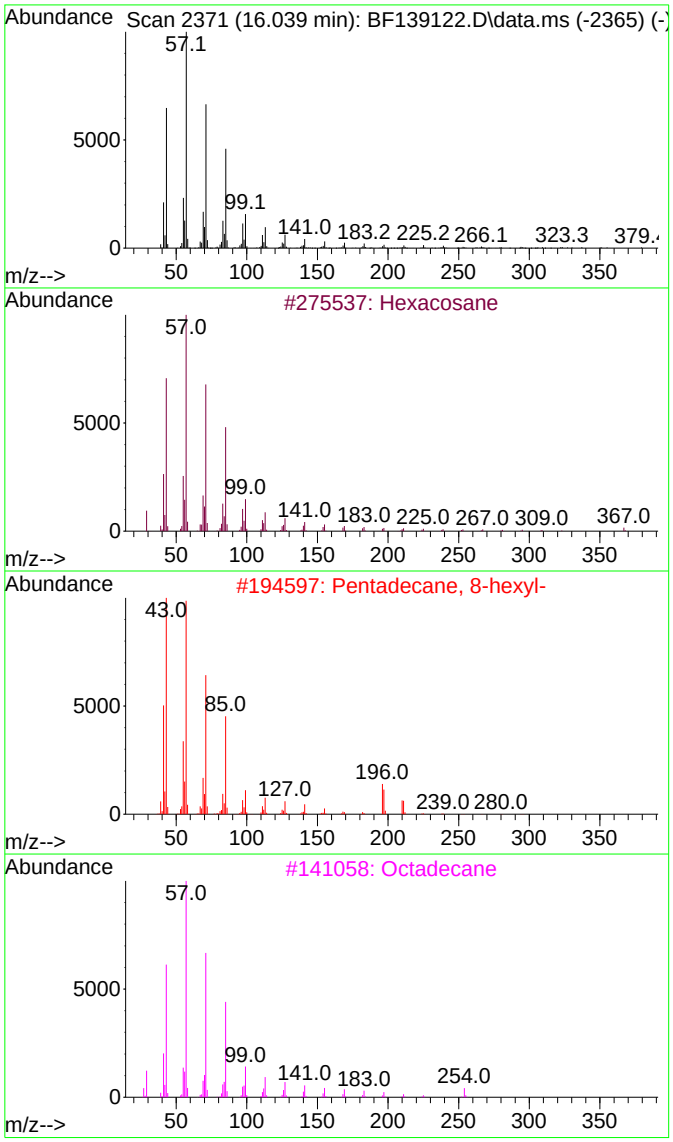
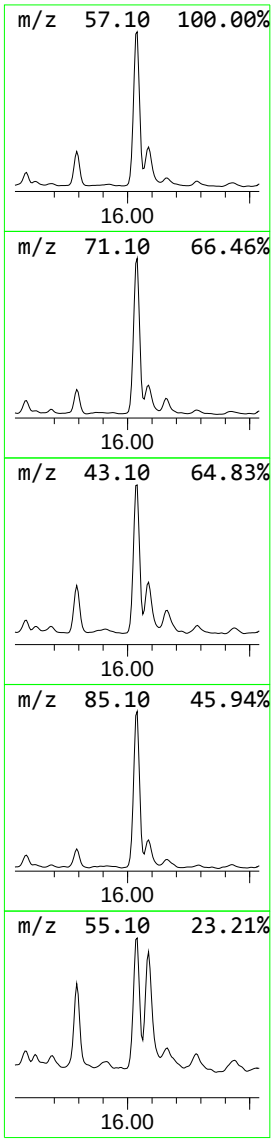
Peak Number 14 Hexacosane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.039	33.37 ng	551027	Perylene-d12	15.533

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosane	366	C26H54	000630-01-3	94
2	Pentadecane, 8-hexyl-	296	C21H44	013475-75-7	94
3	Octadecane	254	C18H38	000593-45-3	93
4	Eicosane, 10-methyl-	296	C21H44	054833-23-7	93
5	Octadecane, 2-methyl-	268	C19H40	001560-88-9	93





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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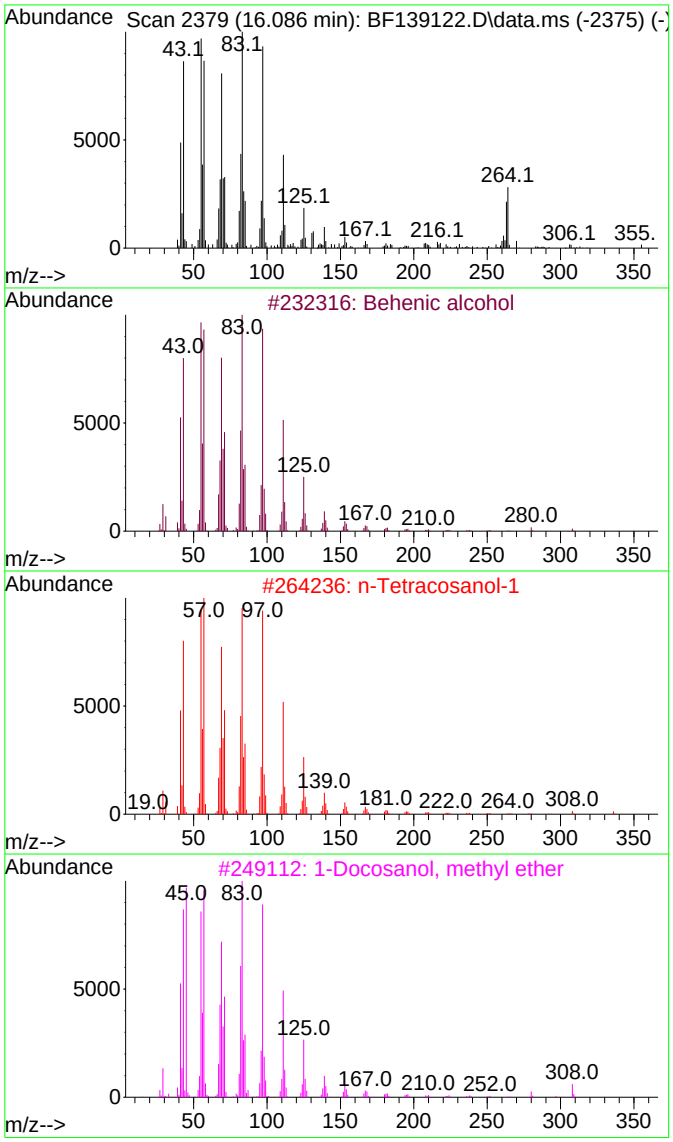
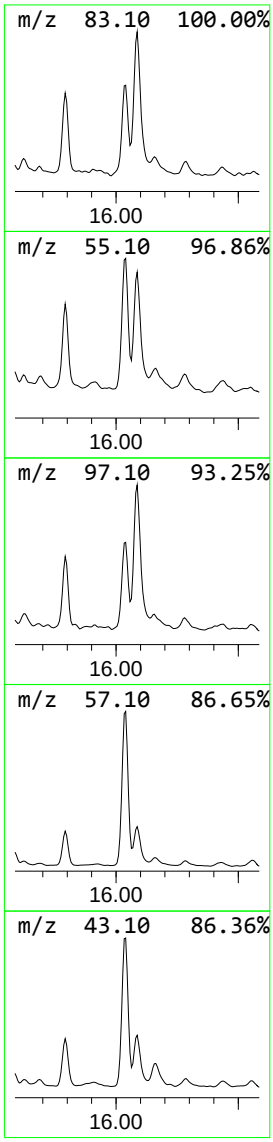
Peak Number 15 Behenic alcohol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.086	18.71 ng	308995	Perylene-d12	15.533

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Behenic alcohol	326	C22H46O	000661-19-8	93
2	n-Tetracosanol-1	354	C24H50O	000506-51-4	91
3	1-Docosanol, methyl ether	340	C23H48O	1000333-91-9	86
4	Cyclopentadecane	210	C15H30	000295-48-7	64
5	1-Docosene	308	C22H44	001599-67-3	55





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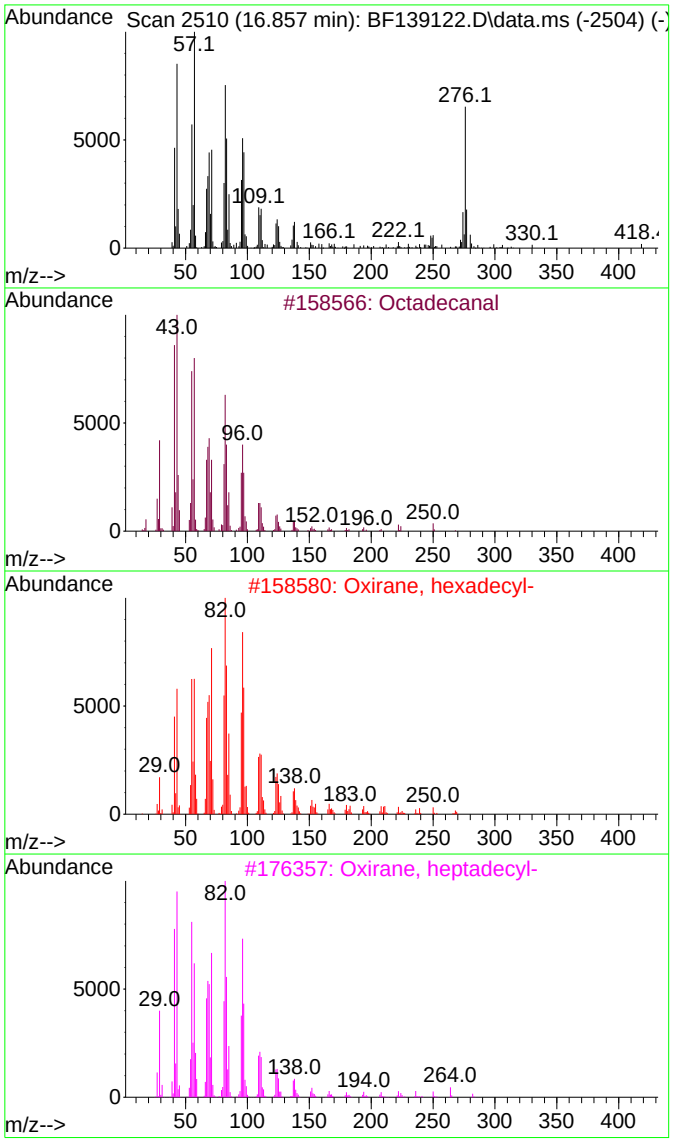
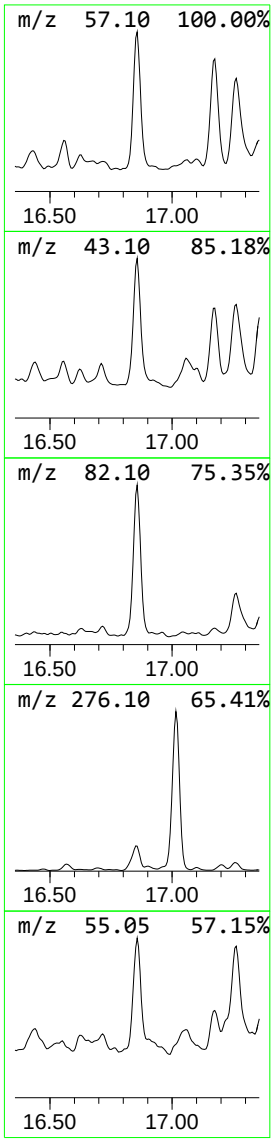
Peak Number 16 Octadecanal Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.857	17.35 ng	286441	Perylene-d12	15.533

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanal	268	C18H36O	000638-66-4	93
2	Oxirane, hexadecyl-	268	C18H36O	007390-81-0	92
3	Oxirane, heptadecyl-	282	C19H38O	067860-04-2	81
4	Hexacosanal	380	C26H52O	026627-85-0	76
5	Eicosanal-	296	C20H40O	002400-66-0	70





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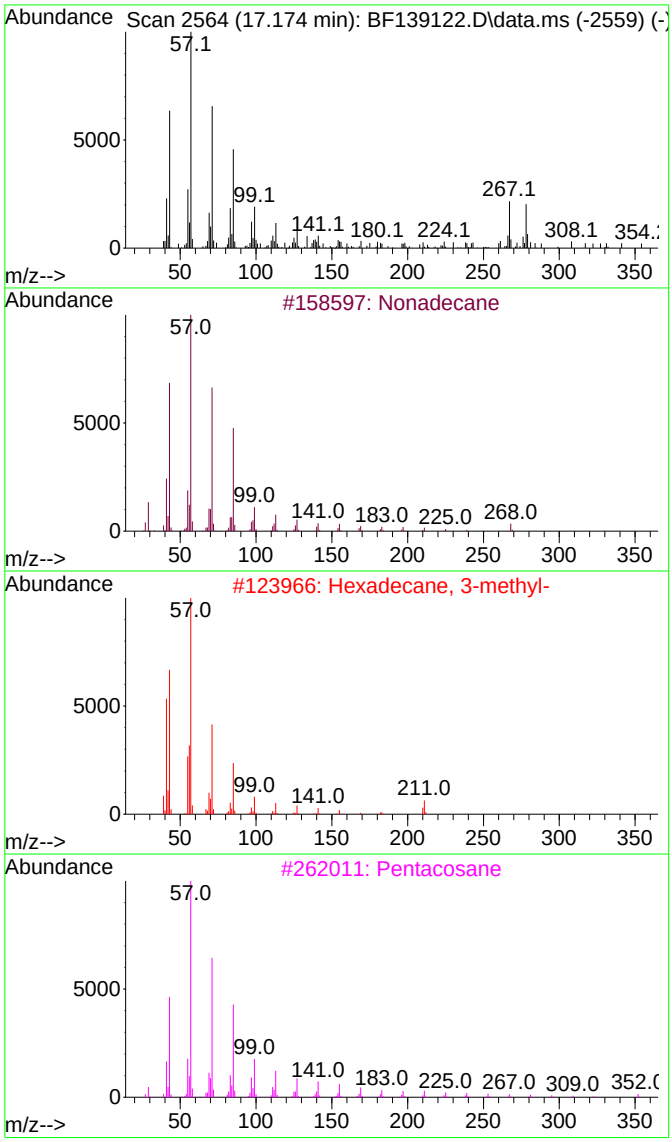
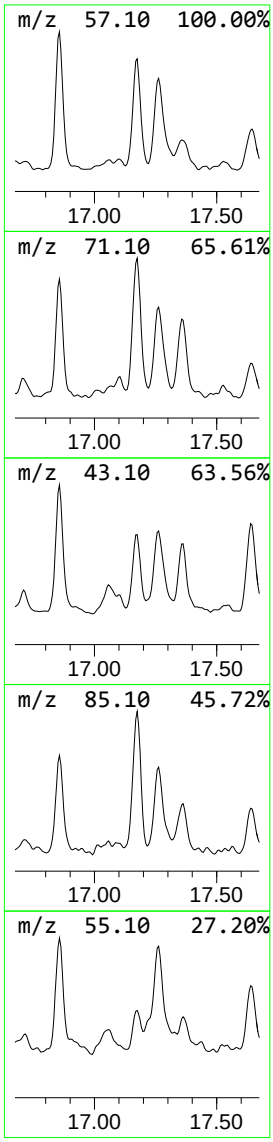
Peak Number 17 Nonadecane Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.174	6.94 ng	114518	Perylene-d12	15.533

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonadecane	268	C19H40	000629-92-5	92
2	Hexadecane, 3-methyl-	240	C17H36	006418-43-5	58
3	Pentacosane	352	C25H52	000629-99-2	58
4	Hentriacontane	437	C31H64	000630-04-6	58
5	Octacosane, 2-methyl-	408	C29H60	001560-98-1	58





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Data File : BF139122.D
Acq On : 22 Aug 2024 14:50
Operator : RC/JU
Sample : P3641-08
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
S-910-K1-0.5-1.0-081524-FD

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

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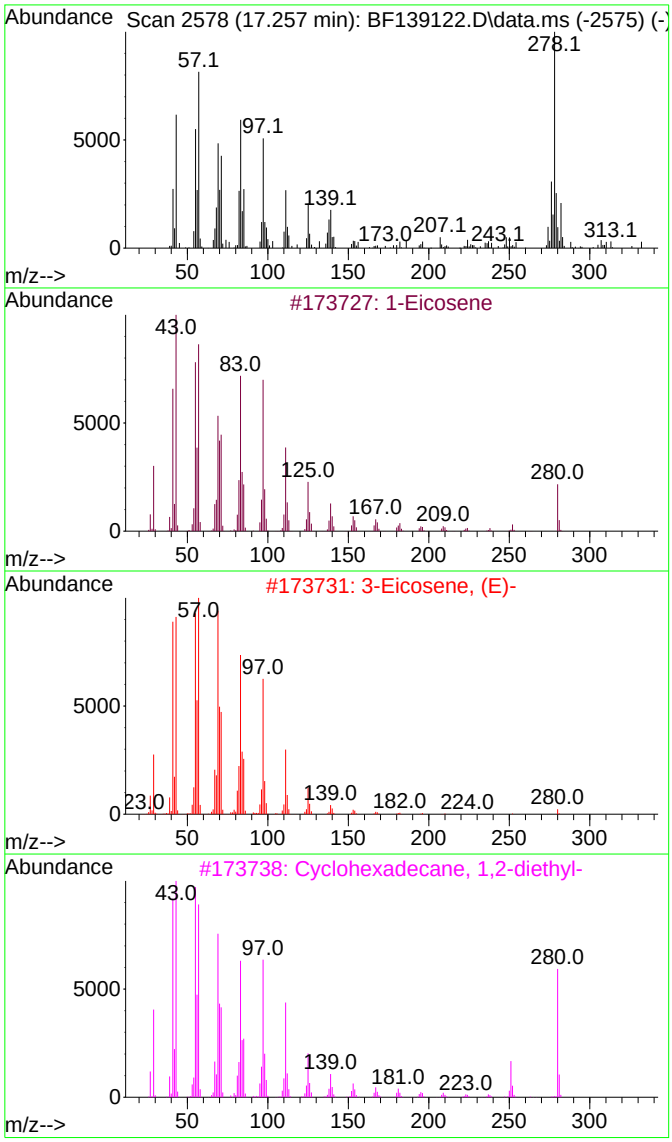
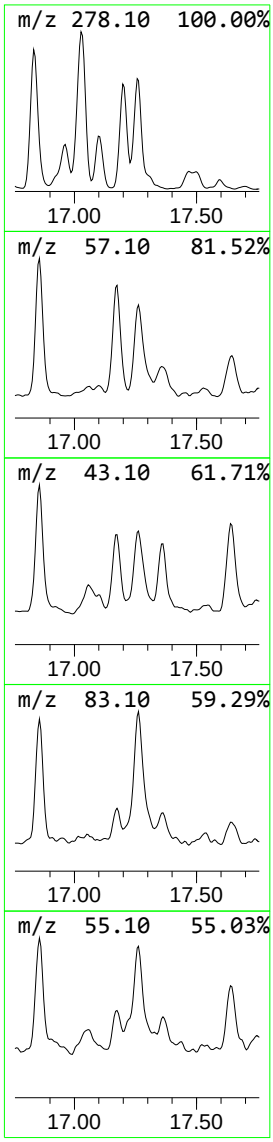
Peak Number 18 1-Eicosene Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.257	12.97 ng	214171	Perylene-d12	15.533

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Eicosene	280	C20H40	003452-07-1	72
2	3-Eicosene, (E)-	280	C20H40	074685-33-9	64
3	Cyclohexadecane, 1,2-diethyl-	280	C20H40	1000155-85-3	62
4	5-Eicosene, (E)-	280	C20H40	074685-30-6	62
5	Pentafluoropropionic acid, hexad...	388	C19H33F5O2	006222-07-7	55





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082224\
Data File : BF139122.D
Acq On : 22 Aug 2024 14:50
Operator : RC/JU
Sample : P3641-08
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
S-910-K1-0.5-1.0-081524-FD

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

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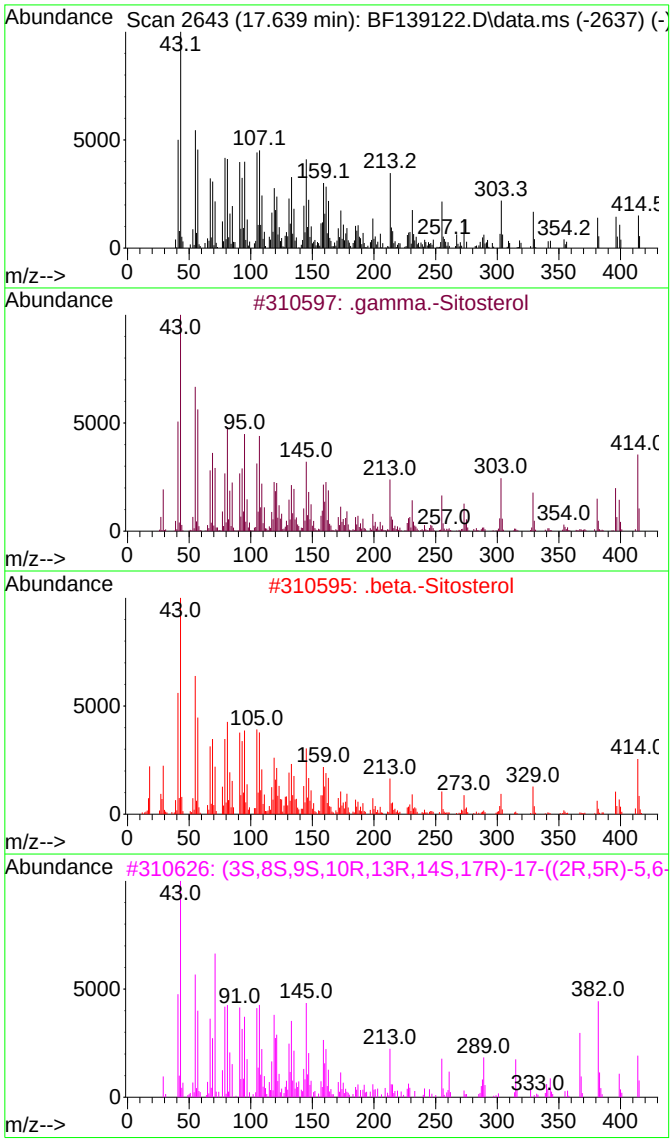
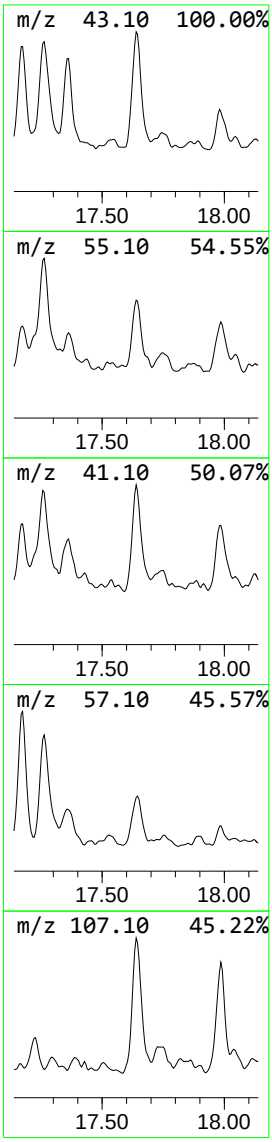
Peak Number 19 .gamma.-Sitosterol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.639	18.27 ng	301648	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	97
3	(3S,8S,9S,10R,13R,14S,17R)-17-((...	414	C29H50O	029365-29-5	55
4	.beta.-Sitosterol acetate	456	C31H52O2	000915-05-9	50
5	5-Cholestene-3-ol, 24-methyl-	400	C28H48O	290299-12-6	49





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082224\
Data File : BF139122.D
Acq On : 22 Aug 2024 14:50
Operator : RC/JU
Sample : P3641-08
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
S-910-K1-0.5-1.0-081524-FD

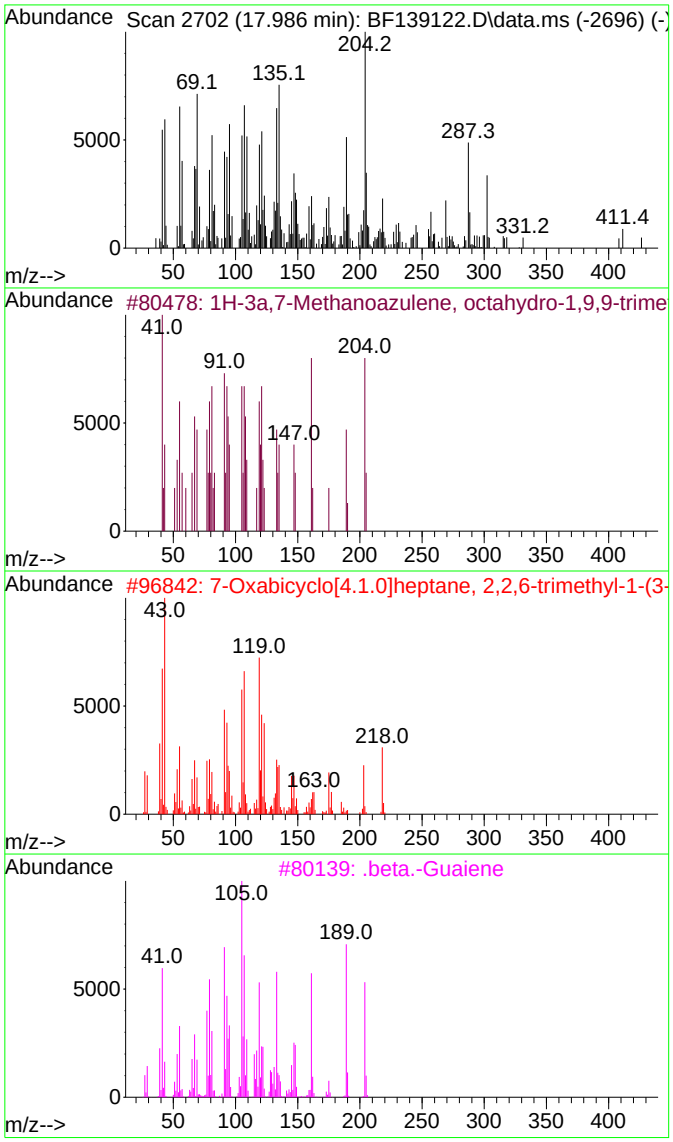
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF082024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

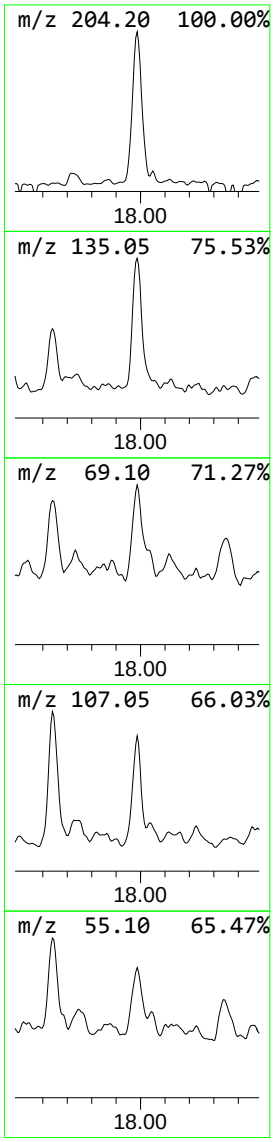
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 20 1H-3a,7-Methanoazulene, oct... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.986	13.29 ng	219532	Perylene-d12	15.533

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-3a,7-Methanoazulene, octahydr...	204	C15H24	000508-55-4	70
2	7-Oxabicyclo[4.1.0]heptane, 2,2,...	218	C15H22O	070038-20-9	53
3	.beta.-Guaiene	204	C15H24	000088-84-6	50
4	2H-Cyclopentacyclooctene, 4,5,6,...	204	C15H24	1000221-85-8	49
5	Naphthalene, decahydro-4a-methyl...	204	C15H24	017066-67-0	49





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082224\
Data File : BF139122.D
Acq On : 22 Aug 2024 14:50
Operator : RC/JU
Sample : P3641-08
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
S-910-K1-0.5-1.0-081524-FD

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

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Butane, 2-metho...	2.187	34.6	ng	883054	1	6.898	510177	20.0
n-Hexadecanoic ...	11.945	12.5	ng	323359	4	11.416	519051	20.0
4H-Cyclopenta[d...	12.028	7.2	ng	187263	4	11.416	519051	20.0
9,10-Anthracene...	12.233	7.4	ng	192312	4	11.416	519051	20.0
11H-Benzo[a]flu...	13.692	4.8	ng	344876	5	14.057	1446230	20.0
1-Docosene	13.904	5.6	ng	405075	5	14.057	1446230	20.0
Cyclopentane, (...	14.539	9.6	ng	691234	5	14.057	1446230	20.0
unknown14.839	14.839	7.6	ng	125143	6	15.533	330260	20.0
Raseglurant, N-...	14.922	5.0	ng	81713	6	15.533	330260	20.0
16-Heptadecenal	14.998	20.2	ng	333789	6	15.533	330260	20.0
Heptafluorobuty...	15.216	68.7	ng	1133940	6	15.533	330260	20.0
Benzo[e]pyrene	15.410	24.7	ng	408208	6	15.533	330260	20.0
Hexacosanal	15.792	14.1	ng	232962	6	15.533	330260	20.0
Hexacosane	16.039	33.4	ng	551027	6	15.533	330260	20.0
Behenic alcohol	16.086	18.7	ng	308995	6	15.533	330260	20.0
Octadecanal	16.857	17.4	ng	286441	6	15.533	330260	20.0
Nonadecane	17.174	6.9	ng	114518	6	15.533	330260	20.0
1-Eicosene	17.257	13.0	ng	214171	6	15.533	330260	20.0
.gamma.-Sitosterol	17.639	18.3	ng	301648	6	15.533	330260	20.0
1H-3a,7-Methano...	17.986	13.3	ng	219532	6	15.533	330260	20.0