LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF021319\
Data File : BF112550.D
Acq On : 13 Feb 2019 20:33
Operator : JU/SJ
Sample : K1458-04
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-2

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-BF012519.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.051	501	504	520	rVB	64402	87070	3.89%	0.425%
2	5.475	572	576	598	rBV	1691354	1918045	85.73%	9.358%
3	6.486	744	748	766	rBV	1904515	2120351	94.78%	10.345%
4	6.616	766	770	778	rVV	2377019	2139810	95.65%	10.440%
5	6.833	804	807	814	rVB	757543	666655	29.80%	3.253%
6	6.992	830	834	845	rBV	1911315	1625134	72.64%	7.929%
7	7.398	900	903	913	rBV	1177410	1218731	54.48%	5.946%
8	8.122	1022	1026	1032	rBV	832022	776046	34.69%	3.786%
9	8.175	1032	1035	1037	rVB2	31448	35283	1.58%	0.172%
10	8.410	1071	1075	1079	rVB6	22571	25819	1.15%	0.126%
11	8.533	1093	1096	1098	rBV	37595	33663	1.50%	0.164%
12	8.622	1107	1111	1114	rBV2	25364	27652	1.24%	0.135%
13	8.792	1138	1140	1145	rVB5	18440	26916	1.20%	0.131%
14	9.133	1196	1198	1204	rBV3	52114	52175	2.33%	0.255%
15	9.192	1204	1208	1217	rBV	2642253	2237194	100.00%	10.915%
16	9.269	1218	1221	1224	rVB2	53299	55966	2.50%	0.273%
17	9.463	1251	1254	1259	rBV4	24756	28395	1.27%	0.139%
18	9.527	1263	1265	1271	rBV6	22961	43780	1.96%	0.214%
19	9.586	1271	1275	1278	rVV2	201232	204030	9.12%	0.995%
20	9.739	1298	1301	1303	rBV2	32840	31291	1.40%	0.153%
21	9.780	1305	1308	1313	rVB2	48613	52125	2.33%	0.254%
22	9.874	1316	1324	1329	rBV2	898668	857277	38.32%	4.183%
23	9.974	1339	1341	1346	rVB4	21210	28534	1.28%	0.139%
24	10.121	1363	1366	1369	rBV3	34582	34760	1.55%	0.170%
25	10.192	1375	1378	1382	rBV5	28661	48375	2.16%	0.236%
26	10.280	1390	1393	1394	rBV2	33590	31605	1.41%	0.154%
27	10.298	1394	1396	1399	rVB2	39472	31700	1.42%	0.155%
28	10.516	1430	1433	1439	rVB2	53250	68325	3.05%	0.333%
29	10.669	1456	1459	1471	rBV	1115738	1157135	51.72%	5.646%
30	10.786	1474	1479	1486	rVB2	106581	147697	6.60%	0.721%
31	11.251	1555	1558	1564	rVB2	57542	68795	3.08%	0.336%
32	11.368	1574	1578	1581	rBV	715489	720462	32.20%	3.515%
33	11.880	1662	1665	1672	rBV2	128363	169384	7.57%	0.826%
34	12.586	1781	1785	1788	rBV	40388	56420	2.52%	0.275%

LSC Area Percent Report

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Acq On : 13 Feb 2019 20:33
Operator : JU/SJ
Sample : K1458-04
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-2

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-BF012519.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	12.615	1788	1790	1797	rVB5	37684	39432	1.76%	0.192%
36	12.668	1797	1799	1804	rBV4	42030	52392	2.34%	0.256%
37	12.815	1821	1824	1829	rVB3	39446	54719	2.45%	0.267%
38	12.945	1842	1846	1850	rBV	1849706	1629263	72.83%	7.949%
39	13.833	1994	1997	2009	rVB2	161380	216951	9.70%	1.058%
40	14.015	2024	2028	2037	rBV	656316	676498	30.24%	3.301%
41	14.151	2049	2051	2053	rBV2	45626	44509	1.99%	0.217%
42	14.457	2101	2103	2111	rBV2	74086	153062	6.84%	0.747%
43	15.098	2209	2212	2215	rVB	149283	157147	7.02%	0.767%
44	15.474	2273	2276	2277	rBV	75594	86260	3.86%	0.421%
45	15.498	2277	2280	2287	rVB	318708	386537	17.28%	1.886%
46	15.903	2346	2349	2355	rVB2	114422	173140	7.74%	0.845%

Sum of corrected areas: 20496510

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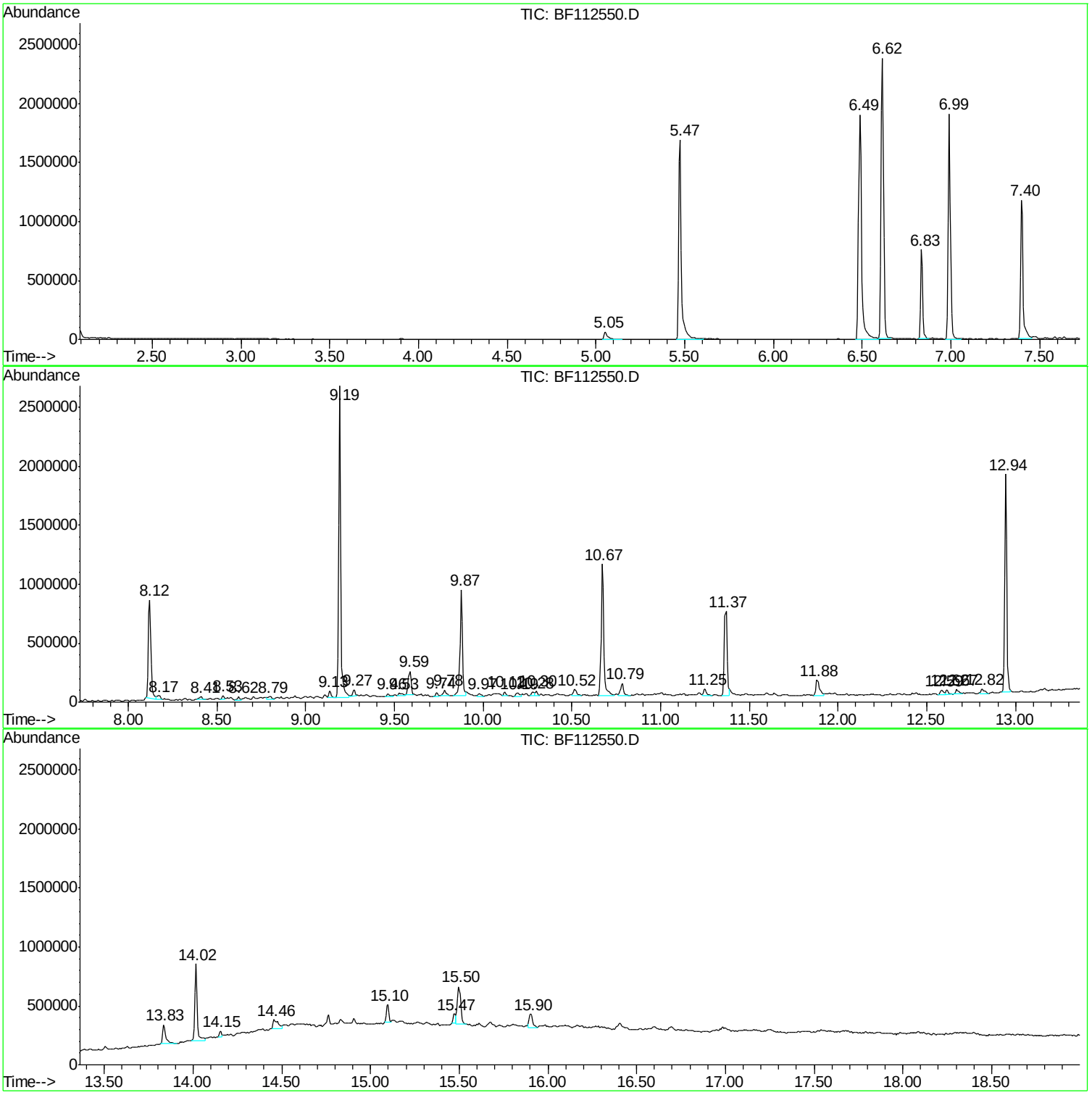
Instrument :
BNA_F
ClientSampleId :
SB-2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF012519.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF021319\
Data File : BF112550.D
Acq On : 13 Feb 2019 20:33
Operator : JU/SJ
Sample : K1458-04
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF012519.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

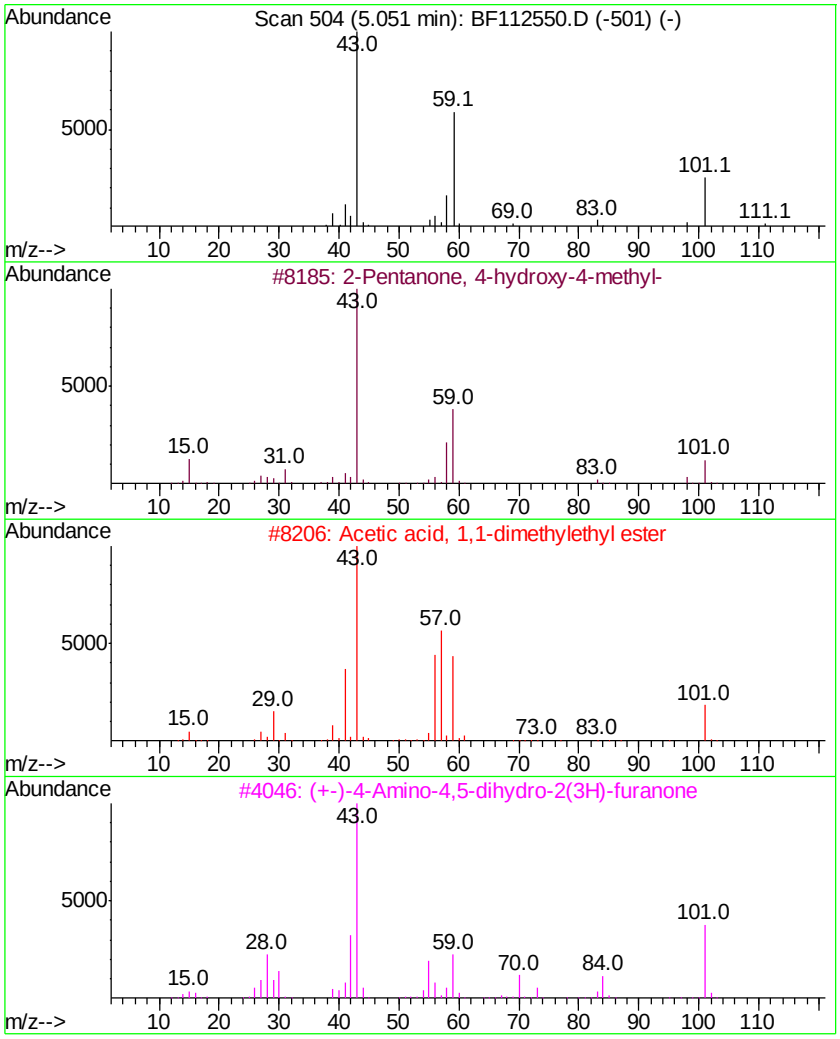
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

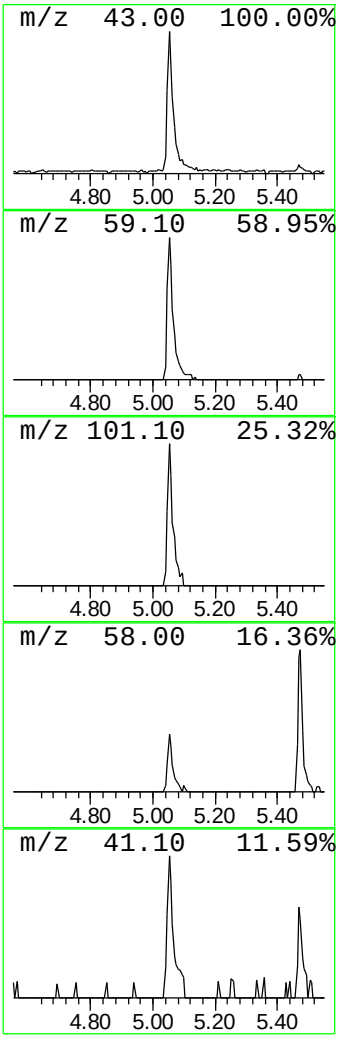
****

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.05	2.61 ng	87070	1,4-Dichlorobenzene-d4	6.83

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3	(+-)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	28
4	3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	27
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF021319\
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Operator : JU/SJ
Sample : K1458-04
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF012519.M
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TIC Library : C:\DATABASE\NIST11.L
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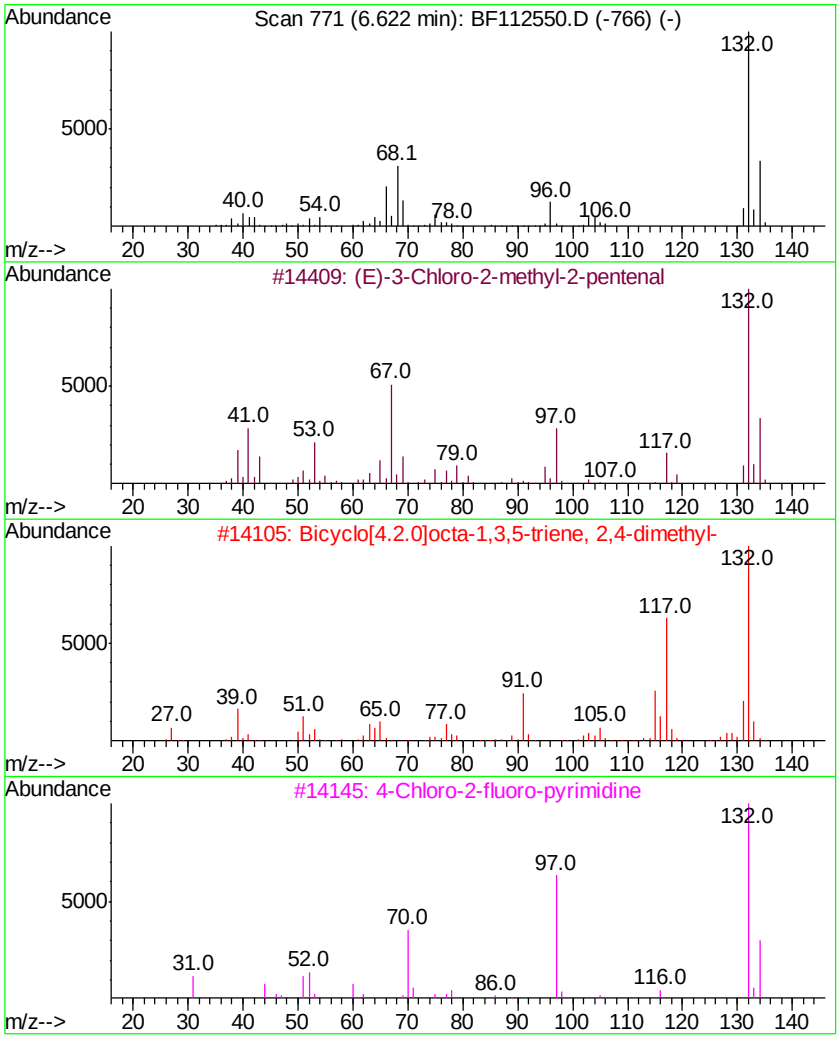
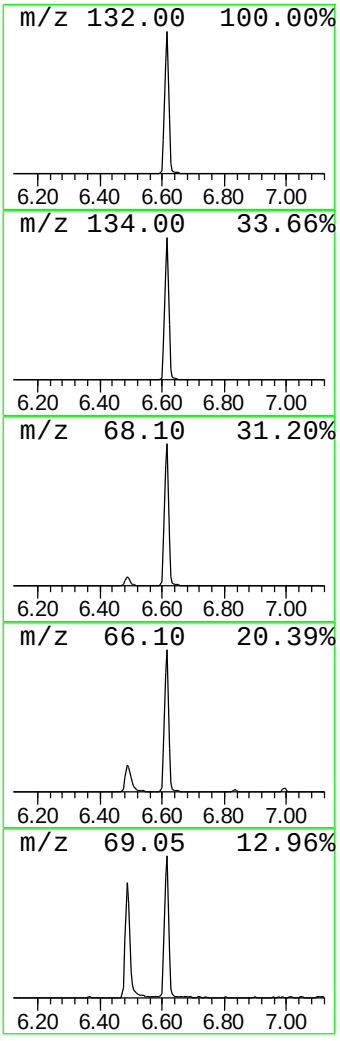
****

Peak Number 2 unknown6.62 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.62	64.20 ng	2139810	1,4-Dichlorobenzene-d4	6.83

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	25
2	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
3	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
4	Cyclopropanamine, 1-phenyl-	133	C9H11N	1000351-26-2	9
5	Xenon	132	Xe	007440-63-3	9





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Sample : K1458-04
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF012519.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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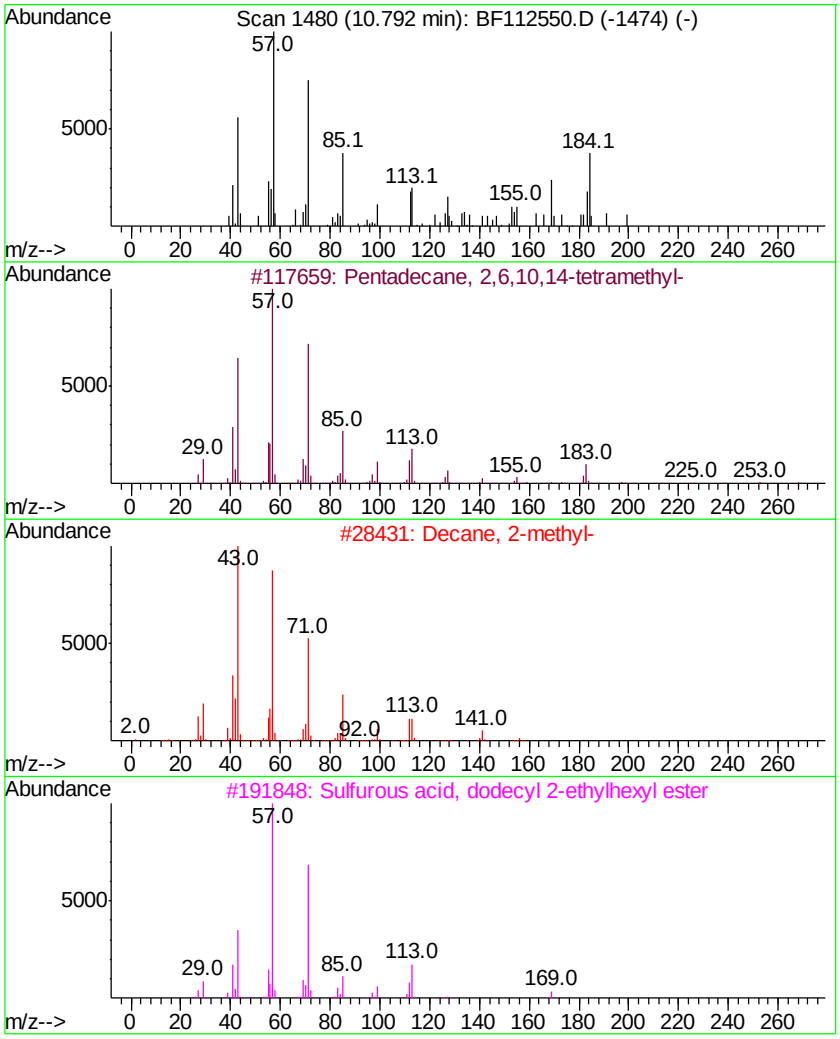
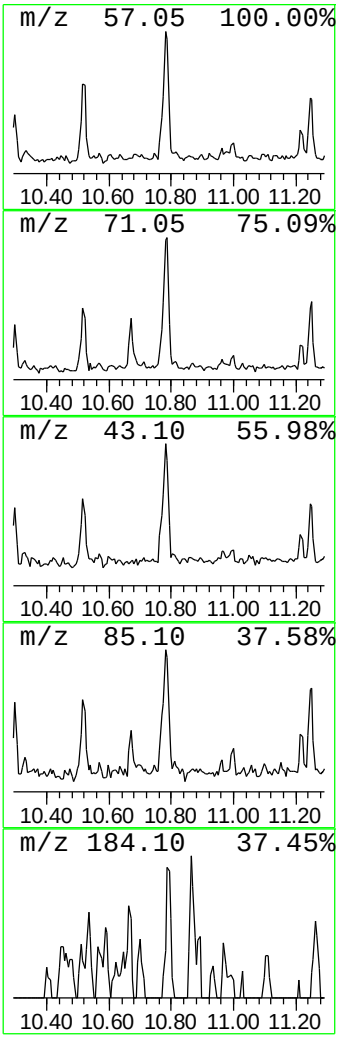
Peak Number 4 Pentadecane, 2,6,10,14-tetr... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.79	4.10 ng	147697	Phenanthrene-d10	11.37

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecane, 2,6,10,14-tetramethyl-	268	C19H40	001921-70-6	87
2	Decane, 2-methyl-	156	C11H24	006975-98-0	74
3	Sulfurous acid, dodecyl 2-ethylh...	362	C20H42O3S	1000309-19-5	72
4	Heptane, 3-ethyl-5-methyl-	142	C10H22	052896-90-9	70
5	Sulfurous acid, 2-ethylhexyl tri...	376	C21H44O3S	1000309-19-6	64





Library Search Compound Report

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Misc :
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Instrument : BNA_F
ClientSampleId : SB-2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF012519.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
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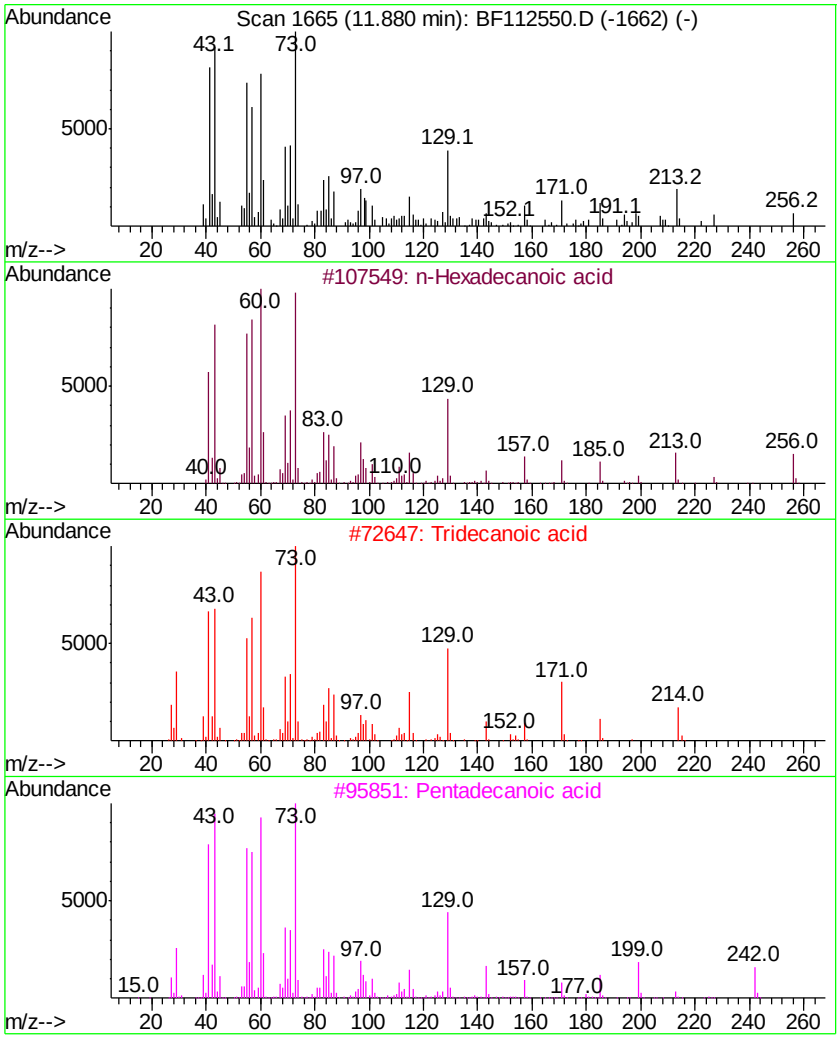
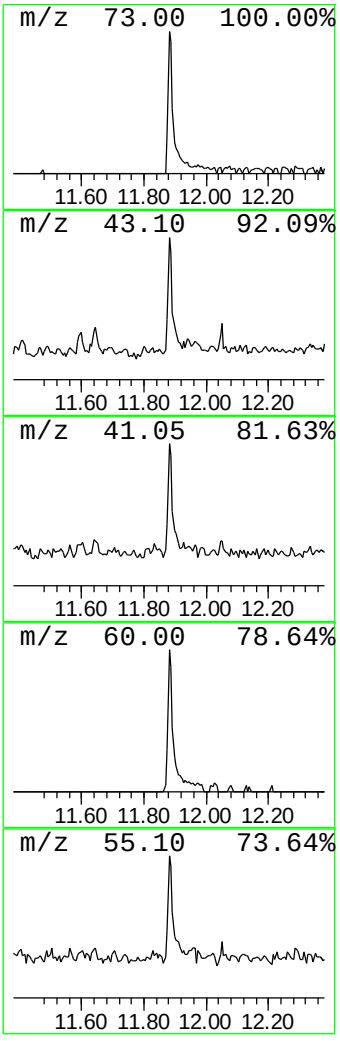
Peak Number 5 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.88	4.70 ng	169384	Phenanthrene-d10	11.37

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	96
2	Tridecanoic acid	214	C13H26O2	000638-53-9	89
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	80
5	n-Decanoic acid	172	C10H20O2	000334-48-5	52





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Misc :
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Instrument : BNA_F
ClientSampleId : SB-2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF012519.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
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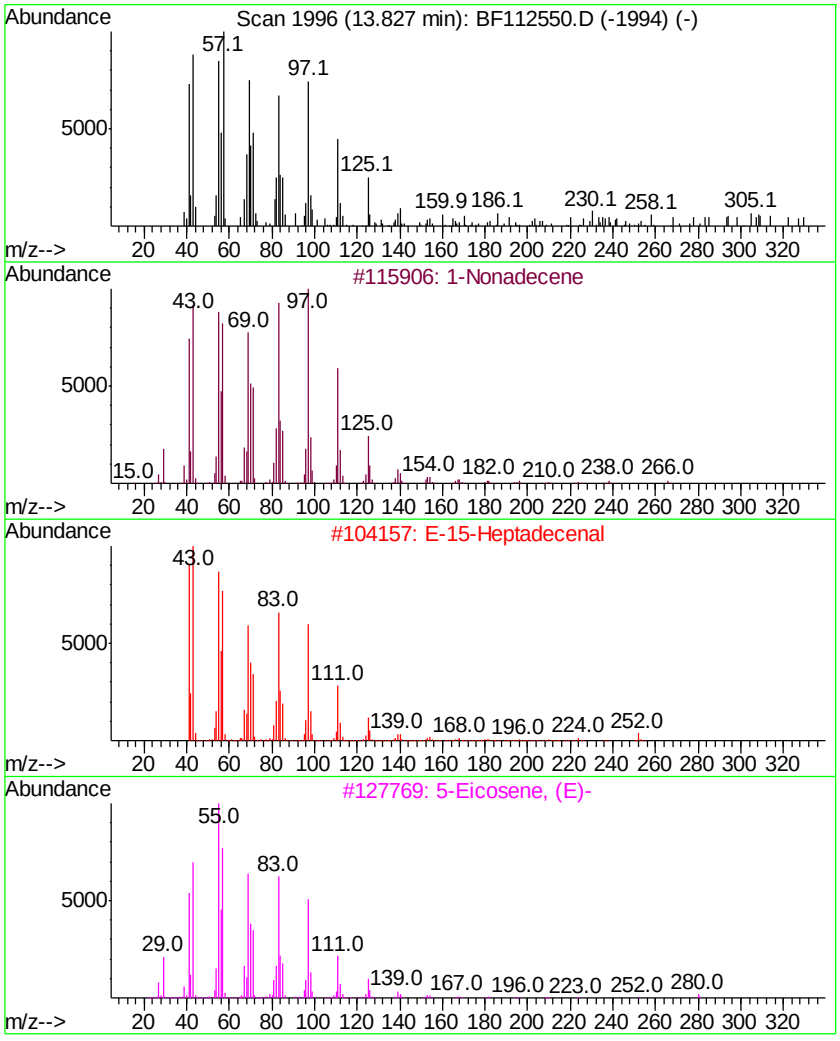
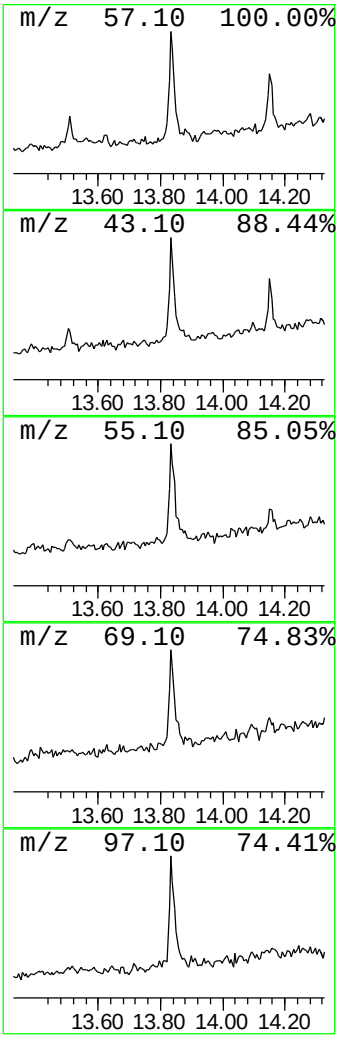
****

Peak Number 6 1-Nonadecene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.83	6.41 ng	216951	Chrysene-d12	14.02

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Nonadecene	266	C19H38	018435-45-5	97
2	E-15-Heptadecenal	252	C17H32O	1000130-97-9	95
3	5-Eicosene, (E)-	280	C20H40	074685-30-6	94
4	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	93
5	1-Docosene	308	C22H44	001599-67-3	91





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Misc :
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ClientSampleId : SB-2

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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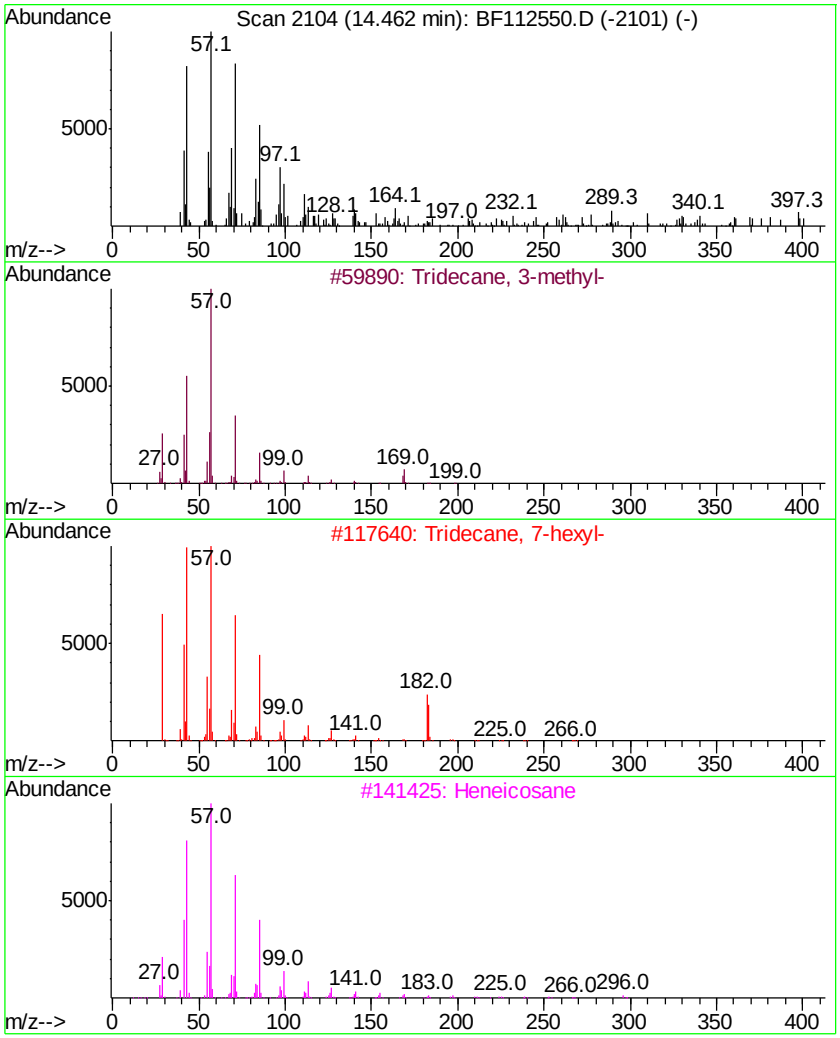
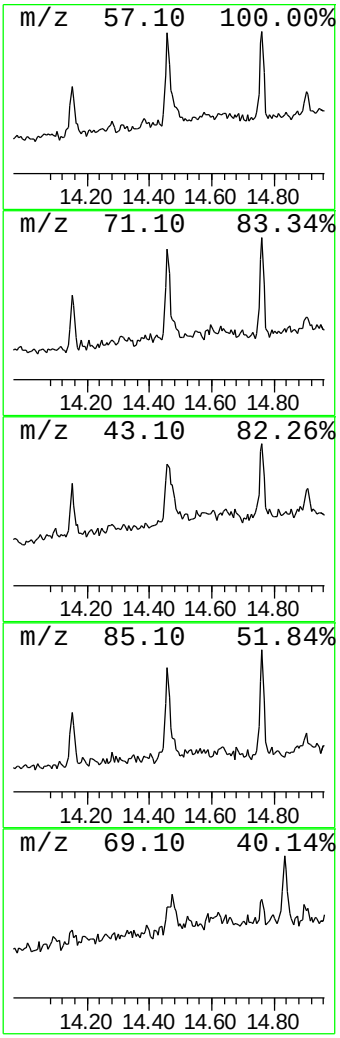
Peak Number 7 Tridecane, 3-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.46	4.53 ng	153062	Chrysene-d12	14.02

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecane, 3-methyl-	198	C14H30	006418-41-3	80
2	Tridecane, 7-hexyl-	268	C19H40	007225-66-3	76
3	Heneicosane	296	C21H44	000629-94-7	64
4	Tetracosane	338	C24H50	000646-31-1	64
5	Pentadecane, 8-hexyl-	296	C21H44	013475-75-7	64





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Instrument : BNA_F
ClientSampleId : SB-2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF012519.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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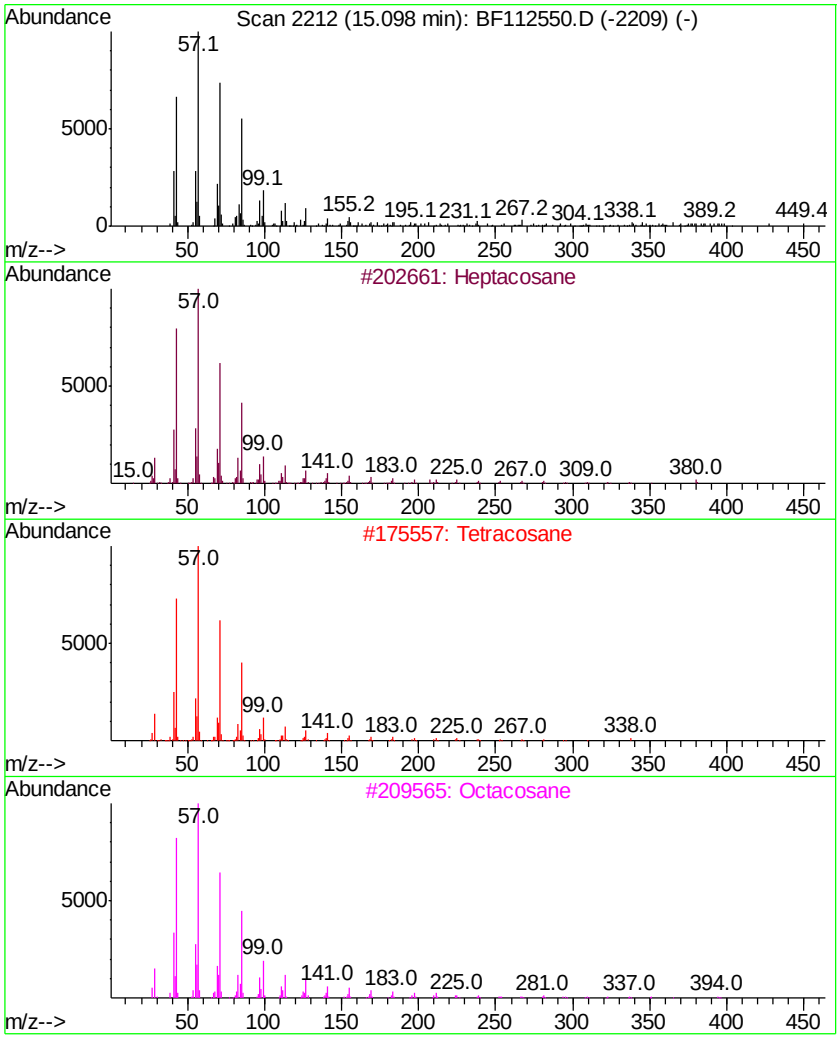
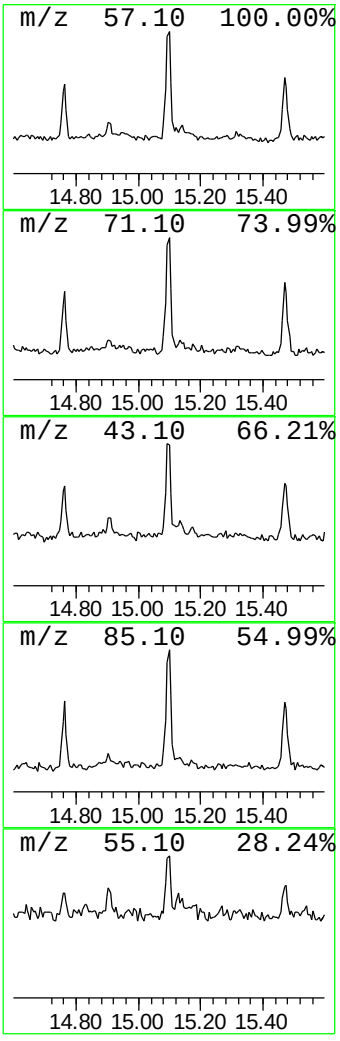
Peak Number 8 Heptacosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.10	8.13 ng	157147	Perylene-d12	15.50

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptacosane	380	C27H56	000593-49-7	95
2	Tetracosane	338	C24H50	000646-31-1	94
3	Octacosane	394	C28H58	000630-02-4	91
4	Tridecane, 1-iodo-	310	C13H27I	035599-77-0	91
5	Eicosane	282	C20H42	000112-95-8	91





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Data File : BF112550.D
Acq On : 13 Feb 2019 20:33
Operator : JU/SJ
Sample : K1458-04
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF012519.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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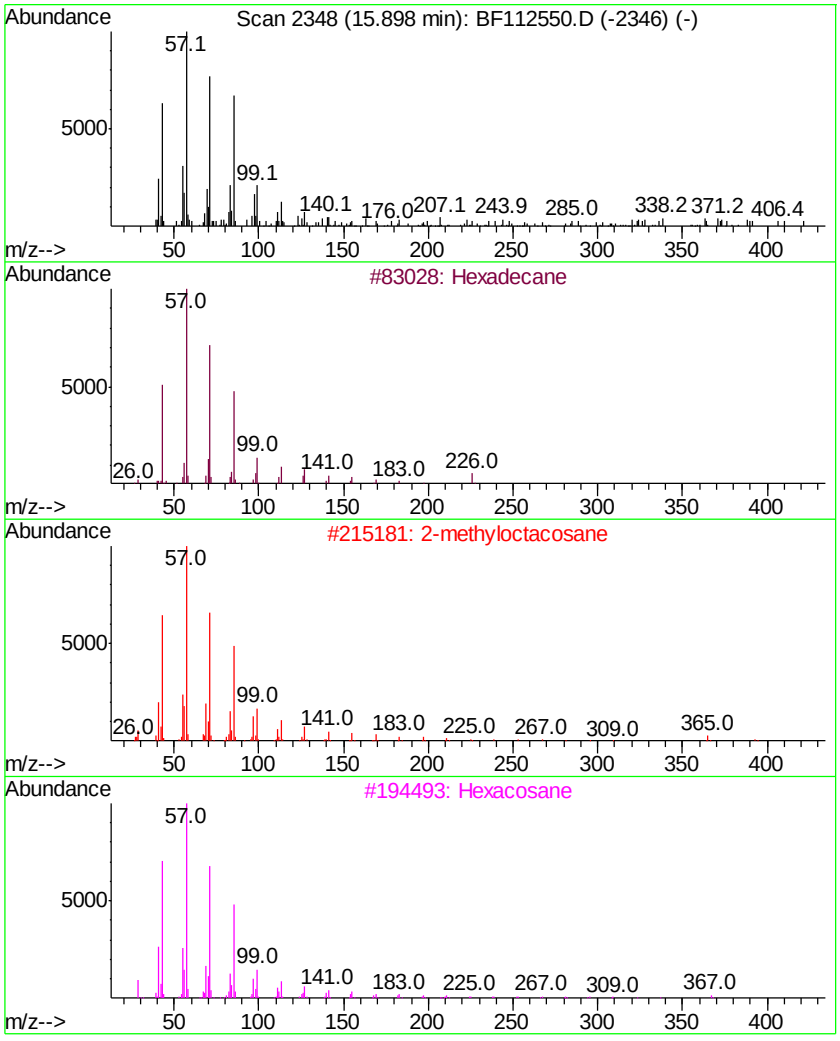
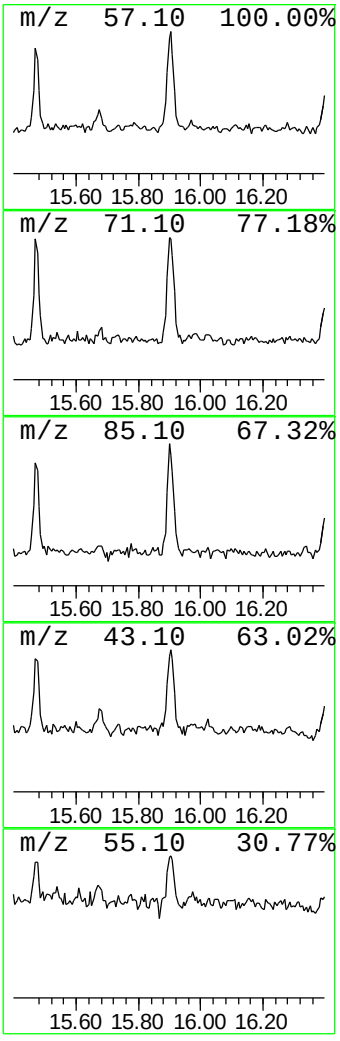
Peak Number 9 Hexadecane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.90	8.96 ng	173140	Perylene-d12	15.50

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	83
2	2-methyloctacosane	408	C29H60	1000376-72-8	81
3	Hexacosane	366	C26H54	000630-01-3	81
4	Tetracosane, 11-decyl-	479	C34H70	055429-84-0	74
5	Tetracosane	338	C24H50	000646-31-1	74





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF021319\
Data File : BF112550.D
Acq On : 13 Feb 2019 20:33
Operator : JU/SJ
Sample : K1458-04
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF012519.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.05	2.6	ng	87070	1	6.83	666655	20.0
unknown6.62	6.62	64.2	ng	2139810	1	6.83	666655	20.0
Pentadecane, 2,6,...	10.79	4.1	ng	147697	4	11.37	720462	20.0
n-Hexadecanoic acid	11.88	4.7	ng	169384	4	11.37	720462	20.0
1-Nonadecene	13.83	6.4	ng	216951	5	14.02	676498	20.0
Tridecane, 3-methyl-	14.46	4.5	ng	153062	5	14.02	676498	20.0
Heptacosane	15.10	8.1	ng	157147	6	15.50	386537	20.0
Hexadecane	15.90	9.0	ng	173140	6	15.50	386537	20.0