LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF020719\
Data File : BF112437.D
Acq On : 7 Feb 2019 14:50
Operator : JU/SJ
Sample : K1389-07
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : M-6

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	517	rVB	105330	147601	4.19%	0.444%
2	5.469	571	575	587	rBV	2859484	2750817	78.07%	8.277%
3	6.481	743	747	760	rBV	2800141	3006784	85.34%	9.047%
4	6.610	765	769	772	rBV	3592375	3082596	87.49%	9.276%
5	6.834	803	807	813	rVB	873066	847066	24.04%	2.549%
6	6.987	829	833	837	rBV	2690137	2462561	69.89%	7.410%
7	7.104	848	853	856	rVB5	38359	48548	1.38%	0.146%
8	7.222	870	873	876	rBV3	32896	38290	1.09%	0.115%
9	7.392	898	902	912	rVB	1775503	1862840	52.87%	5.605%
10	7.469	912	915	919	rVB4	45760	65242	1.85%	0.196%
11	7.528	919	925	926	rBV5	28383	48061	1.36%	0.145%
12	7.751	960	963	967	rVB4	52811	57055	1.62%	0.172%
13	7.798	967	971	973	rBV3	40828	49346	1.40%	0.148%
14	7.863	978	982	984	rBV3	37368	47660	1.35%	0.143%
15	8.051	1012	1014	1019	rBV6	26679	45372	1.29%	0.137%
16	8.116	1019	1025	1030	rVV	1052094	1148826	32.61%	3.457%
17	8.169	1030	1034	1037	rVV2	100052	133576	3.79%	0.402%
18	8.198	1037	1039	1047	rVB8	41002	64813	1.84%	0.195%
19	8.404	1069	1074	1078	rBV6	36301	48526	1.38%	0.146%
20	8.534	1092	1096	1098	rBV	33893	39055	1.11%	0.118%
21	9.186	1202	1207	1218	rBV	3940422	3523379	100.00%	10.602%
22	9.581	1270	1274	1282	rVB	223454	224597	6.37%	0.676%
23	9.869	1319	1323	1327	rBV	1303710	1138348	32.31%	3.425%
24	10.663	1454	1458	1468	rBV	2127169	2108124	59.83%	6.343%
25	10.780	1473	1478	1483	rVB6	34697	61729	1.75%	0.186%
26	11.245	1554	1557	1562	rVB4	27111	38723	1.10%	0.117%
27	11.357	1572	1576	1578	rBV	1157910	1033220	29.32%	3.109%
28	11.380	1578	1580	1586	rVB	152929	145175	4.12%	0.437%
29	11.433	1586	1589	1592	rBV	83920	76455	2.17%	0.230%
30	11.698	1629	1634	1638	rBV2	60393	87407	2.48%	0.263%
31	11.880	1658	1665	1672	rBV3	248099	435145	12.35%	1.309%
32	11.969	1677	1680	1687	rVB	116519	163482	4.64%	0.492%
33	12.433	1757	1759	1763	rBV3	36103	44963	1.28%	0.135%
34	12.569	1779	1782	1786	rBV	651180	602628	17.10%	1.813%

LSC Area Percent Report

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Operator : JU/SJ
Sample : K1389-07
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : M-6

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	12.663	1795	1798	1804	rBV2	72800	91835	2.61%	0.276%
36	12.798	1815	1821	1828	rBV	600516	722542	20.51%	2.174%
37	12.939	1840	1845	1848	rBV	2889797	2658351	75.45%	7.999%
38	13.127	1875	1877	1881	rVB	83451	76444	2.17%	0.230%
39	13.198	1886	1889	1891	rVB	72577	62336	1.77%	0.188%
40	13.233	1892	1895	1900	rBV3	50438	65003	1.84%	0.196%
41	13.357	1914	1916	1918	rBV	49147	50549	1.43%	0.152%
42	13.827	1993	1996	2000	rBV3	293361	312846	8.88%	0.941%
43	13.998	2021	2025	2028	rBV2	975206	1158932	32.89%	3.487%
44	14.027	2028	2030	2033	rVB	251888	211138	5.99%	0.635%
45	14.145	2048	2050	2054	rBV3	90353	96136	2.73%	0.289%
46	14.451	2100	2102	2107	rBV4	113833	143620	4.08%	0.432%
47	14.827	2164	2166	2172	rVB	173533	179587	5.10%	0.540%
48	15.045	2200	2203	2206	rBV	248717	304214	8.63%	0.915%
49	15.351	2252	2255	2260	rVB	164812	188175	5.34%	0.566%
50	15.410	2262	2265	2271	rVB	242395	310744	8.82%	0.935%
51	15.474	2271	2276	2280	rBV	669117	923018	26.20%	2.777%

Sum of corrected areas: 33233480

LSC Report - Integrated Chromatogram

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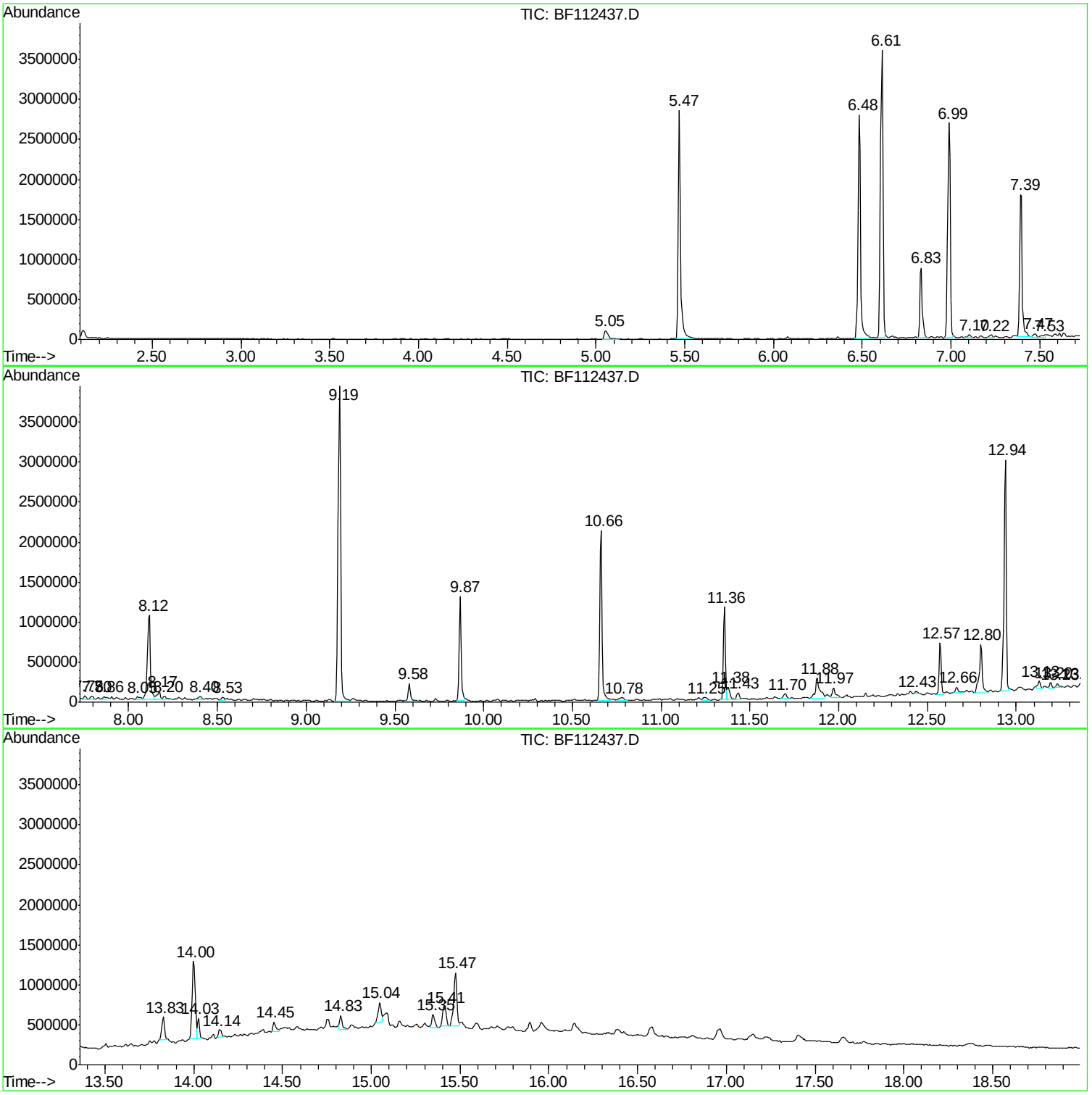
Sample : K1389-07
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : M-6

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



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF020719\
Data File : BF112437.D
Acq On : 7 Feb 2019 14:50
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Sample : K1389-07
Misc :
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Instrument : BNA_F
ClientSampleId : M-6

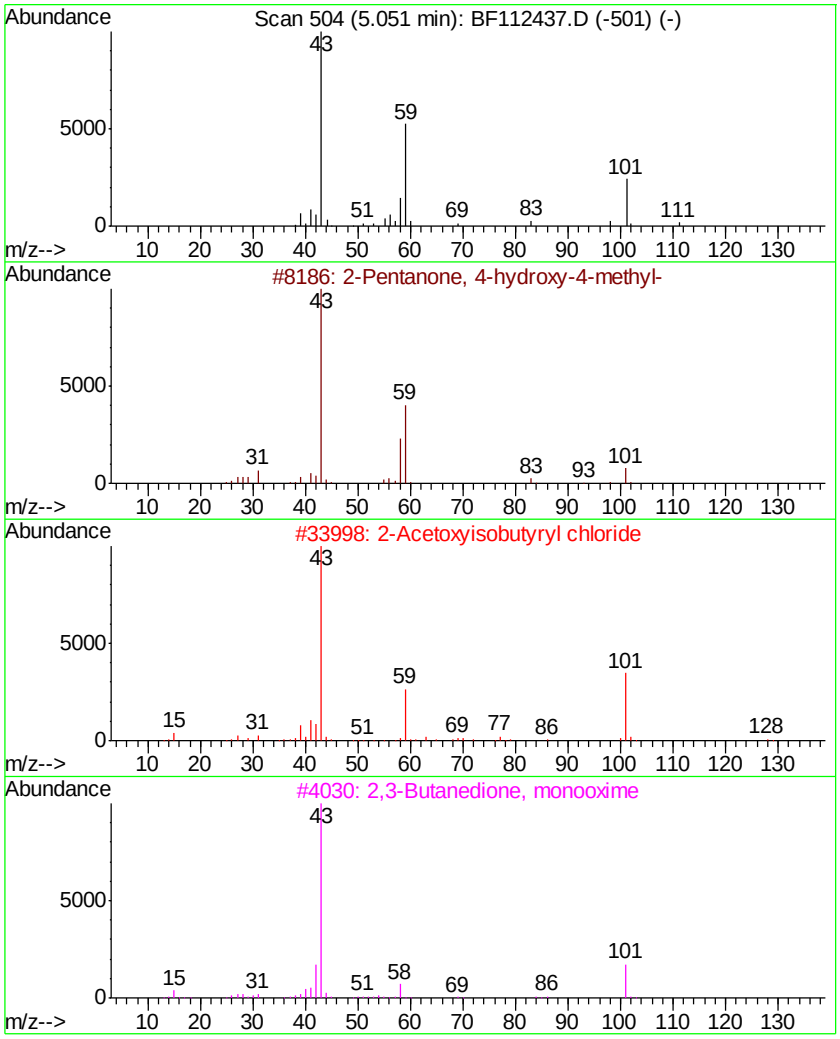
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF012519.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

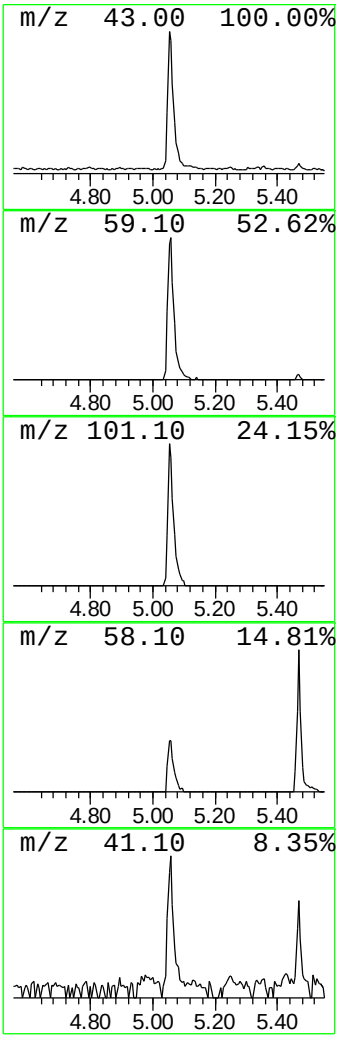
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.05	3.48 ng	147601	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	2-Acetoxyisobutyryl chloride	164	C6H9ClO3	040635-66-3	45
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	35
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
5	Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	17





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Instrument : BNA_F
ClientSampleId : M-6

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

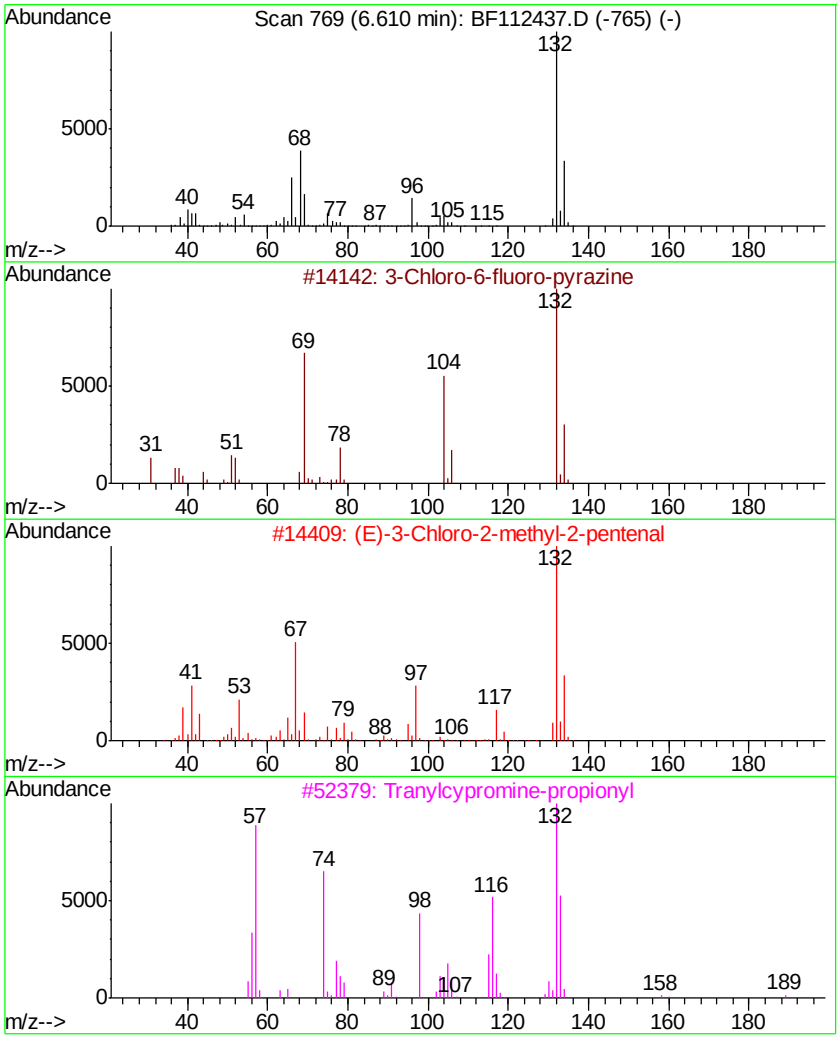
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

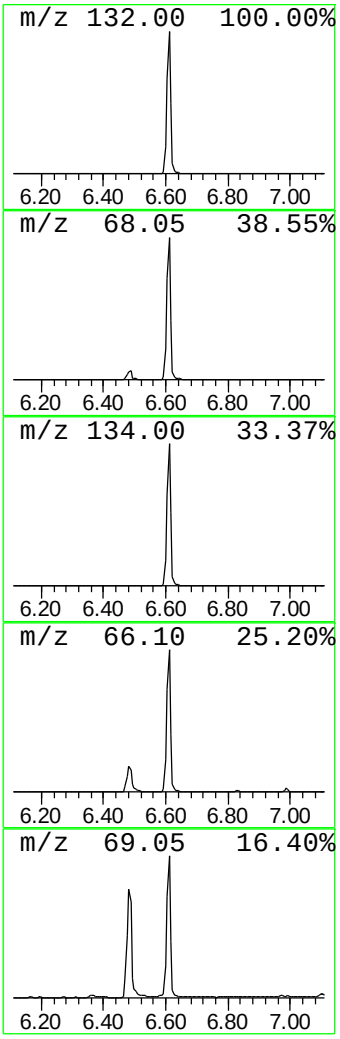
****

Peak Number 2 unknown6.61 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.61	72.78 ng	3082600	1,4-Dichlorobenzene-d4	6.83

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	16
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
4	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF020719\
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Instrument : BNA_F
ClientSampleId : M-6

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

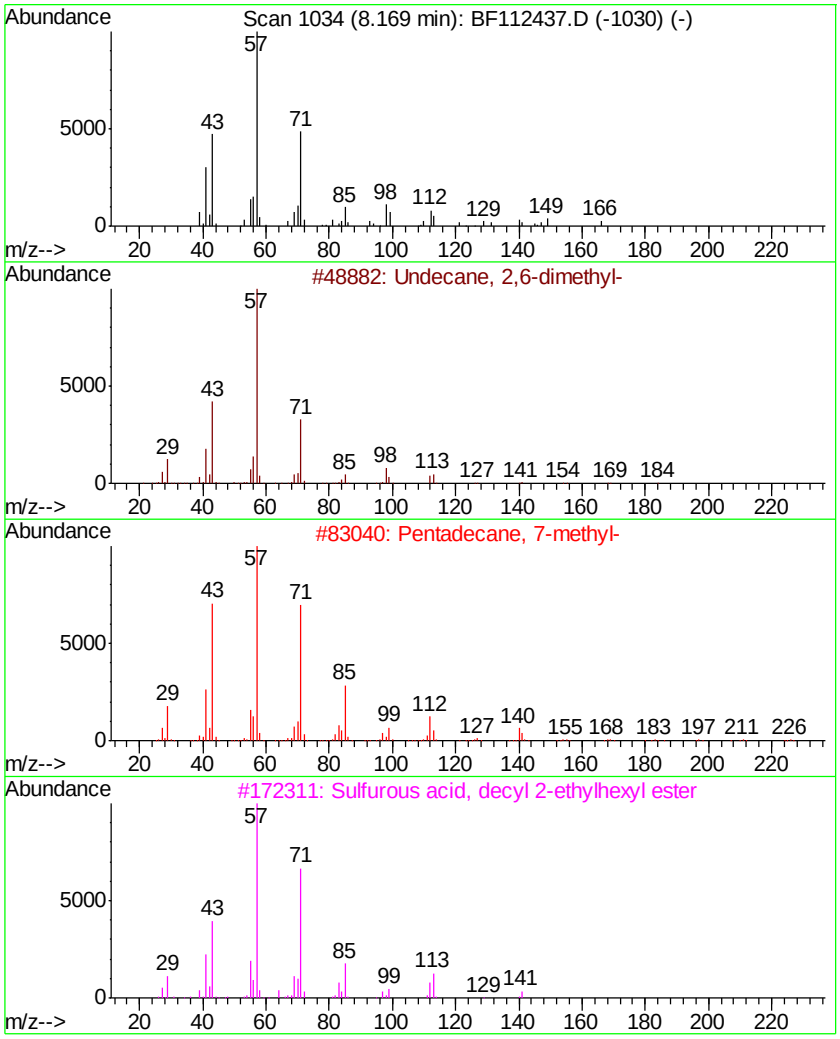
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

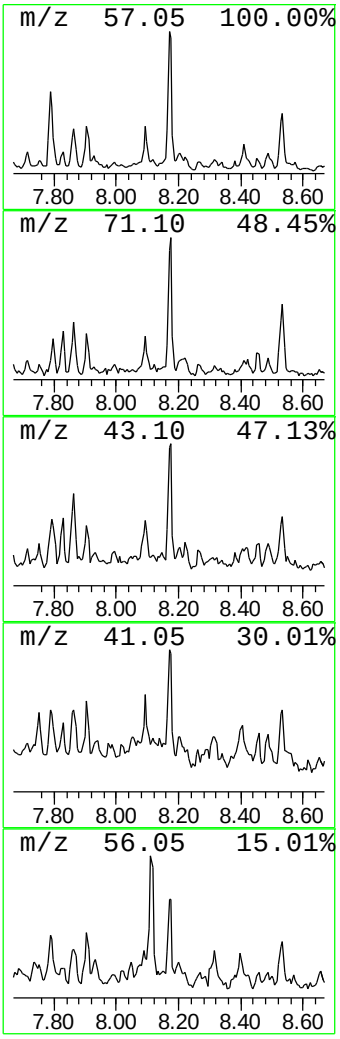
****

Peak Number 4 Undecane, 2,6-dimethyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.17	2.33 ng	133576	Naphthalene-d8	8.12

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Undecane, 2,6-dimethyl-	184	C13H28	017301-23-4	80
2	Pentadecane, 7-methyl-	226	C16H34	006165-40-8	64
3	Sulfurous acid, decyl 2-ethylhex...	334	C18H38O3S	1000309-19-3	59
4	Dodecane, 2,6,10-trimethyl-	212	C15H32	003891-98-3	59
5	Sulfurous acid, 2-ethylhexyl non...	320	C17H36O3S	1000309-19-2	59





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Misc :
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Instrument : BNA_F
ClientSampleId : M-6

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

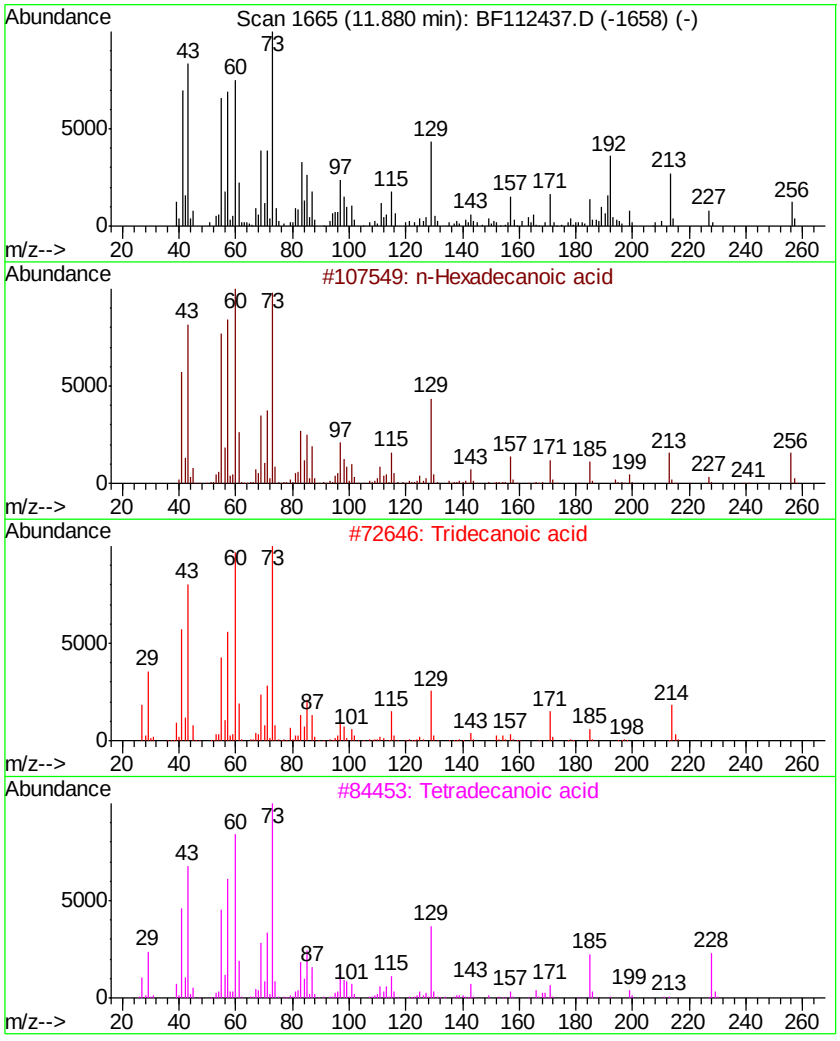
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

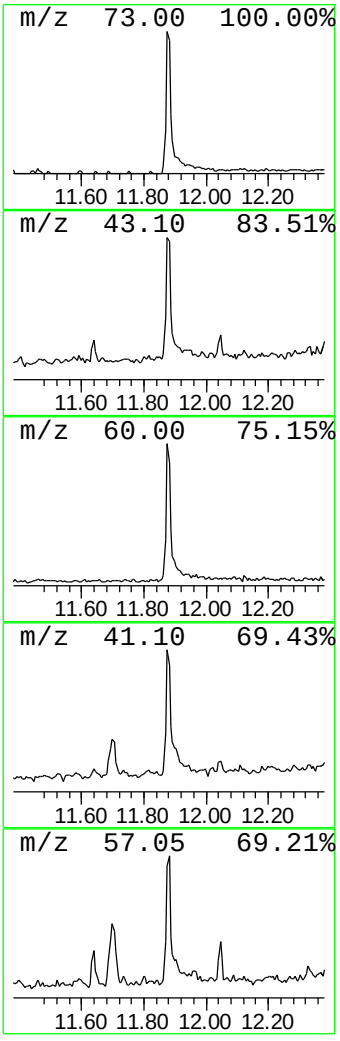
****

Peak Number 5 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.88	8.42 ng	435145	Phenanthrene-d10	11.36

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tridecanoic acid	214	C13H26O2	000638-53-9	91
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	76
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	74
5	n-Decanoic acid	172	C10H20O2	000334-48-5	64





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Instrument : BNA_F
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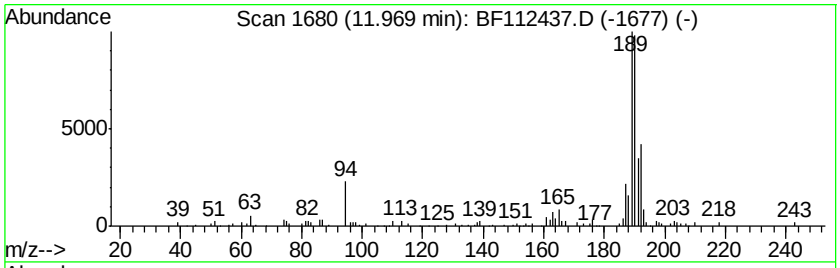
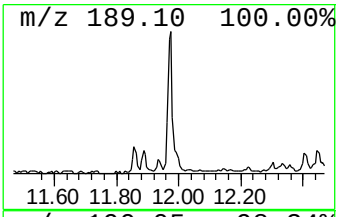
****

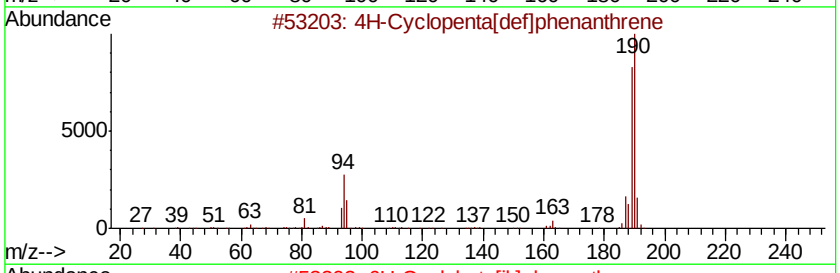
Peak Number 6 4H-Cyclopenta[def]phenanthrene Concentration Rank 8

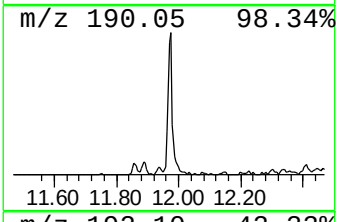
R.T.	EstConc	Area	Relative to ISTD	R.T.
11.97	3.16 ng	163482	Phenanthrene-d10	11.36

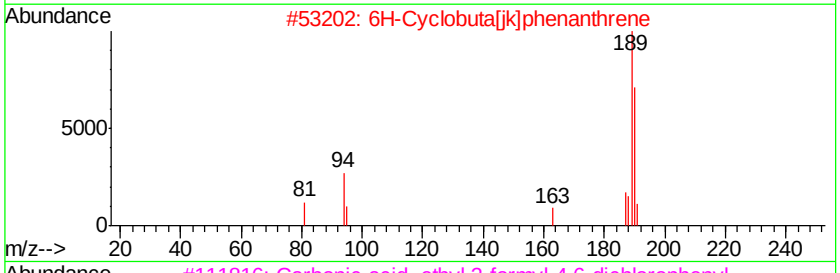
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	64
2	6H-Cyclobuta[jk]phenanthrene	190	C15H10	083469-43-6	59
3	Carbonic acid, ethyl 2-formyl-4,...	262	C10H8Cl2O4	1000331-34-4	40
4	Thiophene-3-carboxaldehyde, 5-ch...	190	C5H4BClO3S	036155-87-0	38
5	Phenol, 4-(2-thienylmethyl)-	190	C11H10OS	091680-55-6	28

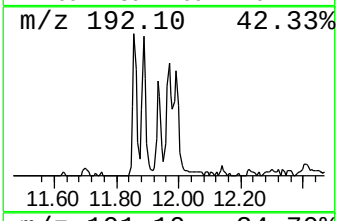


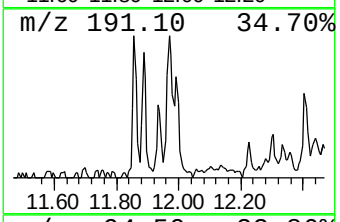


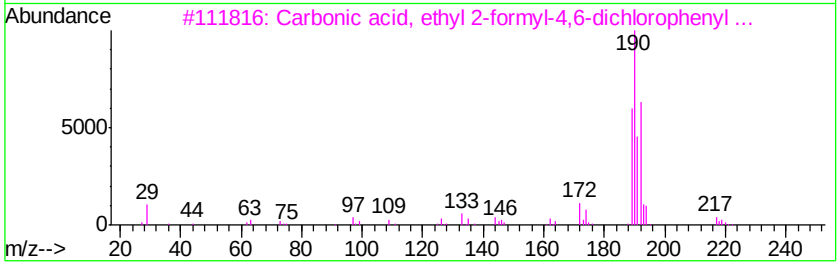


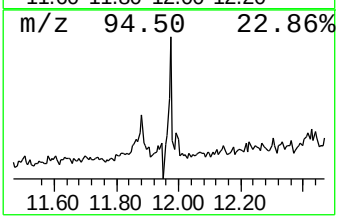












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Misc :
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Instrument : BNA_F
ClientSampleId : M-6

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

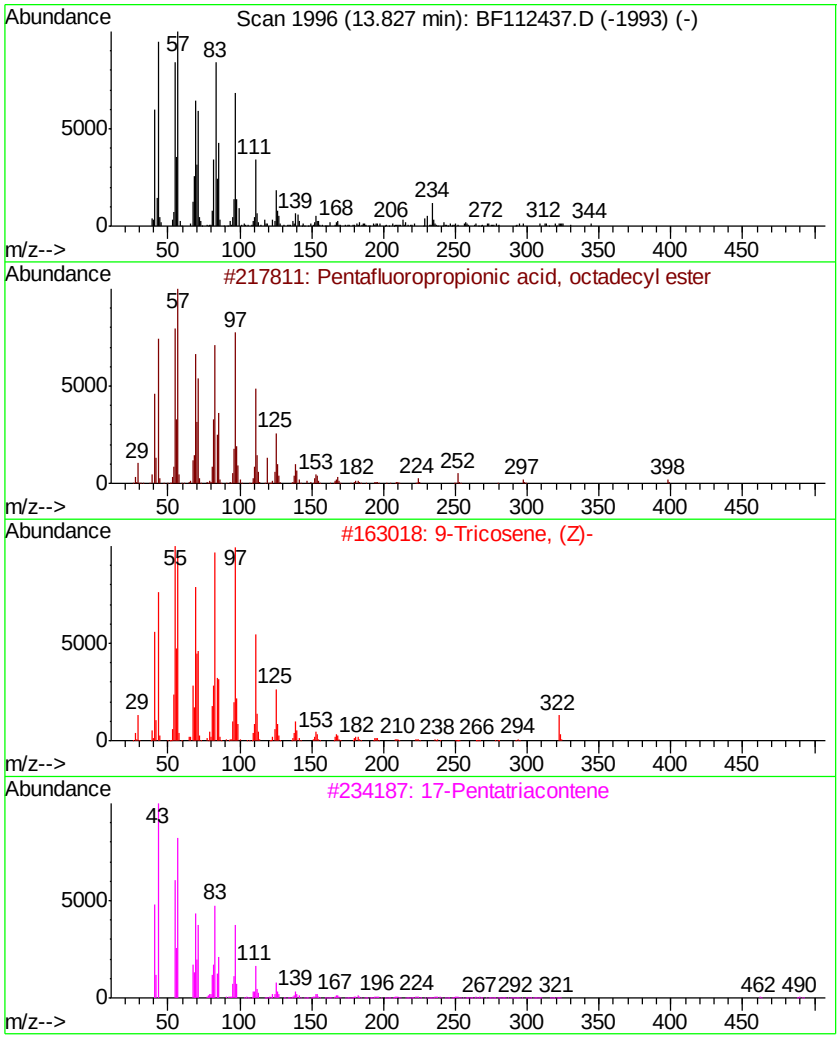
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

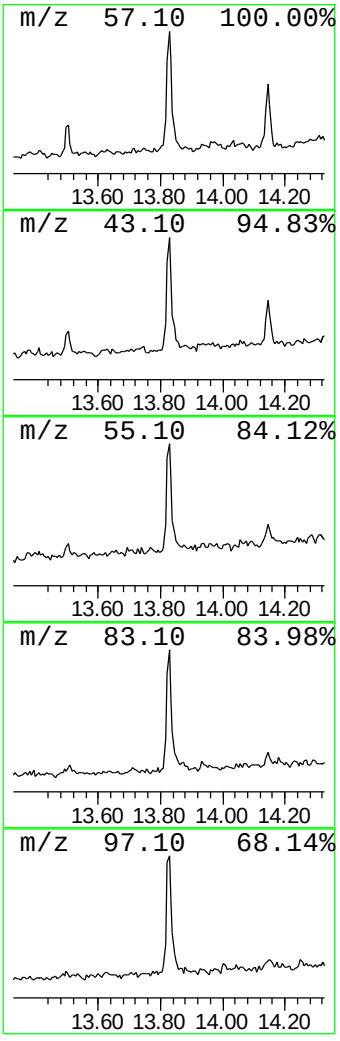
****

Peak Number 7 Pentafluoropropionic acid, ... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.83	5.40 ng	312846	Chrysene-d12	14.00

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentafluoropropionic acid, octad...	416	C21H37F5O2	959261-25-7	91
2	9-Tricosene, (Z)-	322	C23H46	027519-02-4	89
3	17-Pentatriacontene	491	C35H70	006971-40-0	87
4	Behenic alcohol	326	C22H46O	000661-19-8	76
5	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	76





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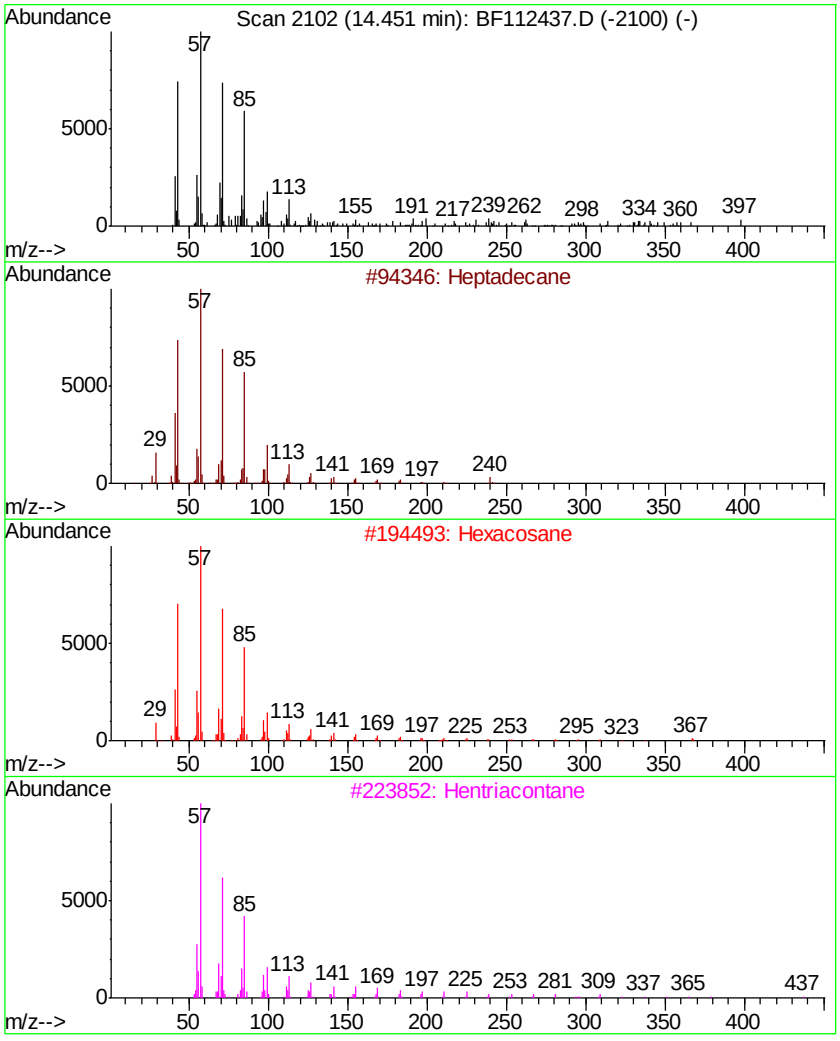
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

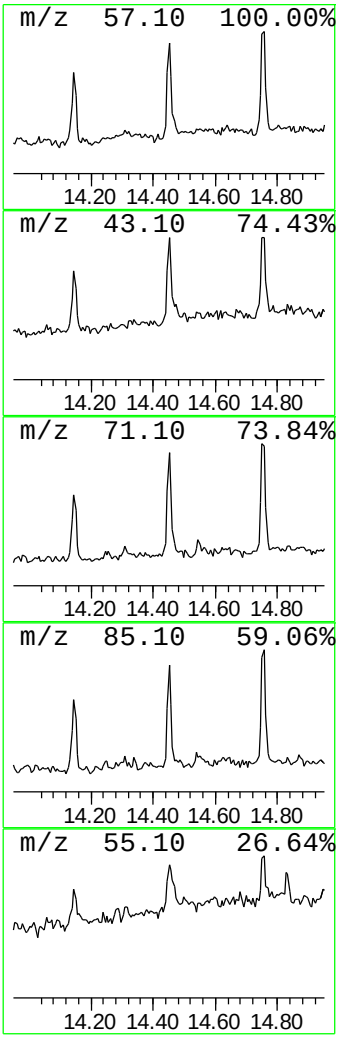
****

Peak Number 8 Heptadecane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.45	2.48 ng	143620	Chrysene-d12	14.00

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane	240	C17H36	000629-78-7	93
2	Hexacosane	366	C26H54	000630-01-3	87
3	Hentriacontane	437	C31H64	000630-04-6	87
4	Heneicosane	296	C21H44	000629-94-7	87
5	Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	86





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF020719\
Data File : BF112437.D
Acq On : 7 Feb 2019 14:50
Operator : JU/SJ
Sample : K1389-07
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : M-6

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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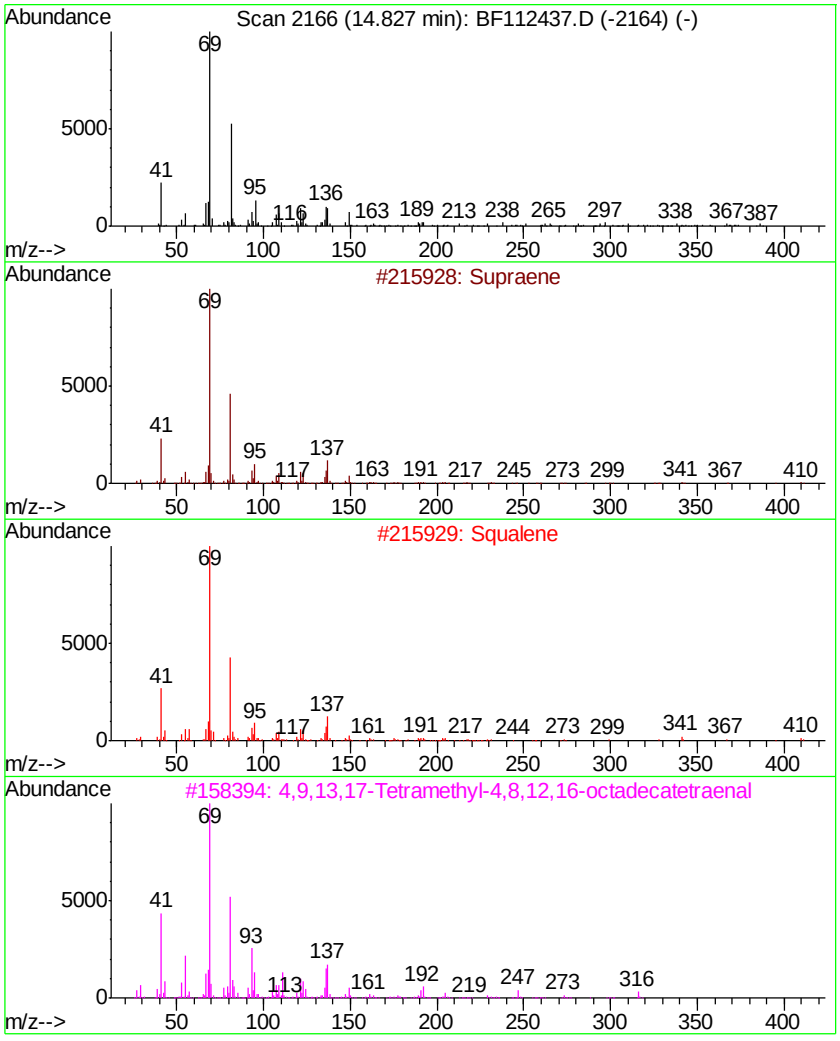
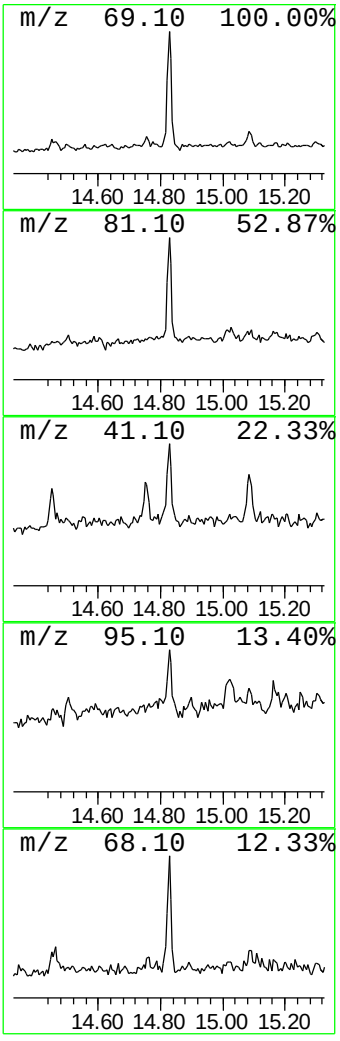
Peak Number 9 Supraene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.83	3.89 ng	179587	Perylene-d12	15.47

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Supraene	410	C30H50	007683-64-9	87
2	Squalene	410	C30H50	000111-02-4	78
3	4,9,13,17-Tetramethyl-4,8,12,16-...	316	C22H36O	056882-09-8	78
4	trans-Farnesol	222	C15H26O	000106-28-5	78
5	7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	72





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF020719\
Data File : BF112437.D
Acq On : 7 Feb 2019 14:50
Operator : JU/SJ
Sample : K1389-07
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : M-6

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	3.5	ng	147601	1	6.83	847066	20.0
unknown6.61	6.61	72.8	ng	3082600	1	6.83	847066	20.0
Undecane, 2,6-dim...	8.17	2.3	ng	133576	2	8.12	1148830	20.0
n-Hexadecanoic acid	11.88	8.4	ng	435145	4	11.36	1033220	20.0
4H-Cyclopenta[def...	11.97	3.2	ng	163482	4	11.36	1033220	20.0
Pentafluoropropio...	13.83	5.4	ng	312846	5	14.00	1158930	20.0
Heptadecane	14.45	2.5	ng	143620	5	14.00	1158930	20.0
Supraene	14.83	3.9	ng	179587	6	15.47	923018	20.0