LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF021319\
Data File : BF112535.D
Acq On : 13 Feb 2019 13:28
Operator : JU/SJ
Sample : K1442-06
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : COMP-12

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	5.045	500	503	516	rVB	60225	79284	4.41%	0.381%
2	5.469	572	575	592	rBV	1461860	1599808	88.99%	7.690%
3	6.486	744	748	764	rBV	1601417	1663602	92.54%	7.996%
4	6.610	766	769	776	rBV	1932981	1797753	100.00%	8.641%
5	6.833	804	807	816	rBV	680859	554371	30.84%	2.665%
6	6.992	830	834	843	rBV	1644586	1416085	78.77%	6.807%
7	7.398	899	903	921	rBV	1154505	1084947	60.35%	5.215%
8	8.116	1022	1025	1046	rVB	727381	699590	38.91%	3.363%
9	9.192	1204	1208	1219	rBV	1819399	1760100	97.91%	8.460%
10	9.586	1272	1275	1283	rVB	108943	120661	6.71%	0.580%
11	9.733	1297	1300	1306	rBV	51528	56633	3.15%	0.272%
12	9.874	1320	1324	1328	rBV	741759	692544	38.52%	3.329%
13	10.292	1389	1395	1399	rVB2	15547	23734	1.32%	0.114%
14	10.421	1414	1417	1423	rVB3	17041	21487	1.20%	0.103%
15	10.669	1455	1459	1470	rBV	1124381	1134137	63.09%	5.451%
16	10.780	1473	1478	1481	rVV4	24488	38126	2.12%	0.183%
17	10.974	1506	1511	1513	rBV6	20155	25681	1.43%	0.123%
18	11.216	1548	1552	1555	rBV	60928	56468	3.14%	0.271%
19	11.363	1573	1577	1579	rBV	763668	663316	36.90%	3.188%
20	11.386	1579	1581	1587	rVB	233764	204662	11.38%	0.984%
21	11.439	1587	1590	1593	rBV	58389	52202	2.90%	0.251%
22	11.604	1613	1618	1622	rBV5	22185	41108	2.29%	0.198%
23	11.639	1622	1624	1629	rVV2	21378	33824	1.88%	0.163%
24	11.698	1632	1634	1639	rVB5	17188	24786	1.38%	0.119%
25	11.880	1659	1665	1673	rBV3	271029	412354	22.94%	1.982%
26	11.945	1673	1676	1679	rVB	28117	23993	1.33%	0.115%
27	11.980	1679	1682	1684	rBV	80605	83761	4.66%	0.403%
28	12.045	1691	1693	1696	rBV2	23522	22382	1.24%	0.108%
29	12.157	1710	1712	1716	rBV	37429	31717	1.76%	0.152%
30	12.198	1717	1719	1723	rVB3	25031	25965	1.44%	0.125%
31	12.415	1753	1756	1758	rBV	52027	47069	2.62%	0.226%
32	12.510	1768	1772	1775	rBV2	42787	57339	3.19%	0.276%
33	12.580	1780	1784	1789	rBV	718627	657054	36.55%	3.158%
34	12.668	1796	1799	1806	rBV3	123438	168284	9.36%	0.809%

LSC Area Percent Report

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Acq On : 13 Feb 2019 13:28
Operator : JU/SJ
Sample : K1442-06
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : COMP-12

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	12.757	1812	1814	1816	rVB3	35334	30283	1.68%	0.146%
36	12.810	1817	1823	1829	rBV	661334	708954	39.44%	3.408%
37	12.945	1842	1846	1849	rVV	1657195	1476995	82.16%	7.099%
38	12.974	1849	1851	1855	rVB2	34100	41383	2.30%	0.199%
39	13.139	1877	1879	1881	rVB	65964	50079	2.79%	0.241%
40	13.204	1888	1890	1892	rBV	47804	30753	1.71%	0.148%
41	13.833	1994	1997	2001	rVB2	235278	232645	12.94%	1.118%
42	14.009	2023	2027	2030	rBV2	798363	1037098	57.69%	4.985%
43	14.039	2030	2032	2035	rVB	293670	242514	13.49%	1.166%
44	14.457	2101	2103	2108	rBV2	98046	113797	6.33%	0.547%
45	15.062	2203	2206	2209	rBV	263603	376812	20.96%	1.811%
46	15.092	2209	2211	2215	rVB2	289586	302724	16.84%	1.455%
47	15.368	2256	2258	2263	rVB	150942	160835	8.95%	0.773%
48	15.433	2267	2269	2273	rVV	186519	213256	11.86%	1.025%
49	15.498	2277	2280	2283	rVB	347485	411912	22.91%	1.980%

Sum of corrected areas: 20804867

LSC Report - Integrated Chromatogram

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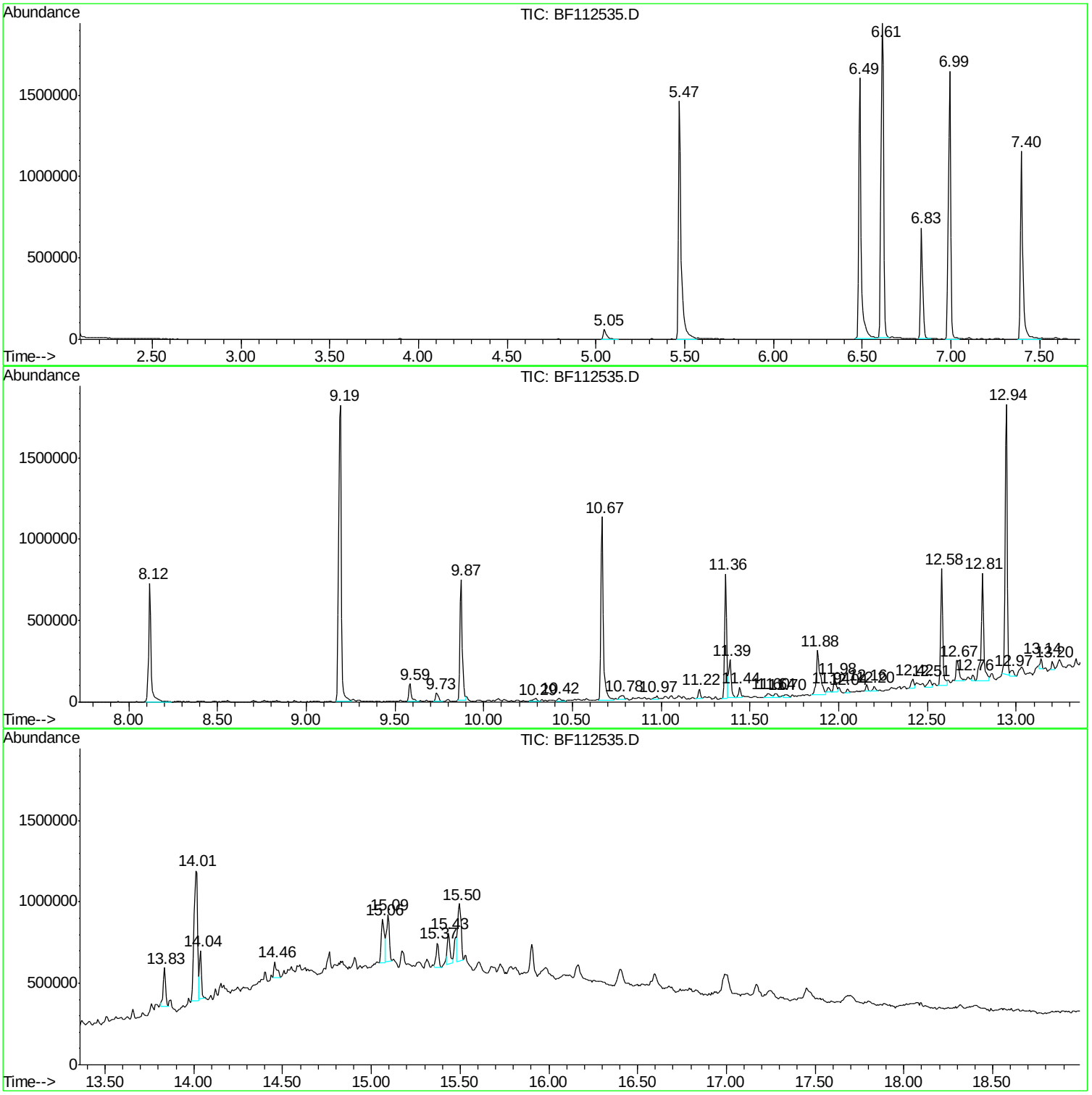
Data File : BF112535.D
Acq On : 13 Feb 2019 13:28
Operator : JU/SJ
Sample : K1442-06
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
COMP-12

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\BF021319\
Data File : BF112535.D
Acq On : 13 Feb 2019 13:28
Operator : JU/SJ
Sample : K1442-06
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : COMP-12

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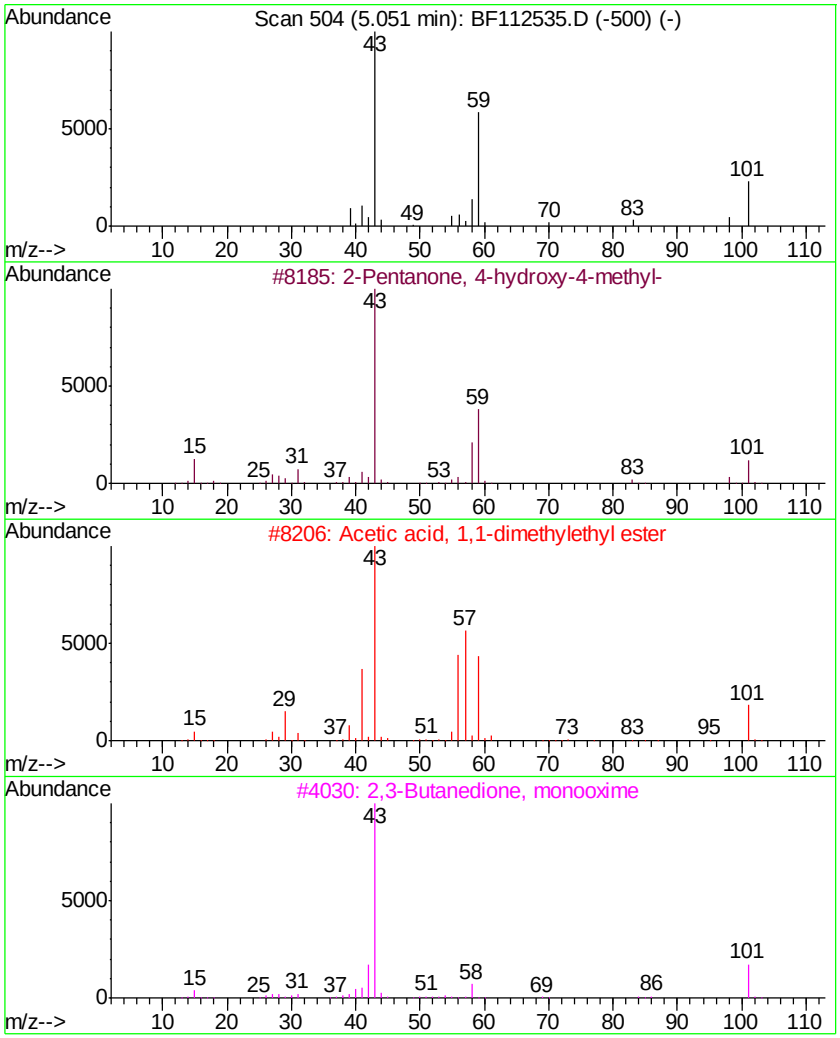
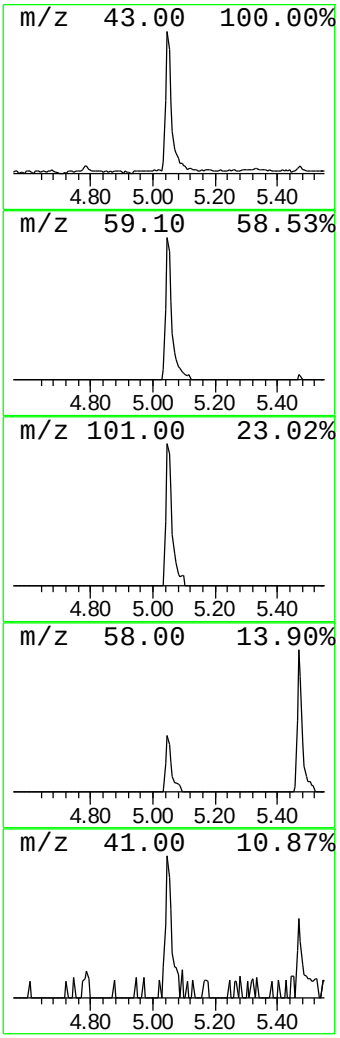
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.05	2.86 ng	79284	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	50
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	35
4	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28
5	2-Nonanone, 9-hydroxy-	158	C9H18O2	025368-56-3	25





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Data File : BF112535.D
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Operator : JU/SJ
Sample : K1442-06
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : COMP-12

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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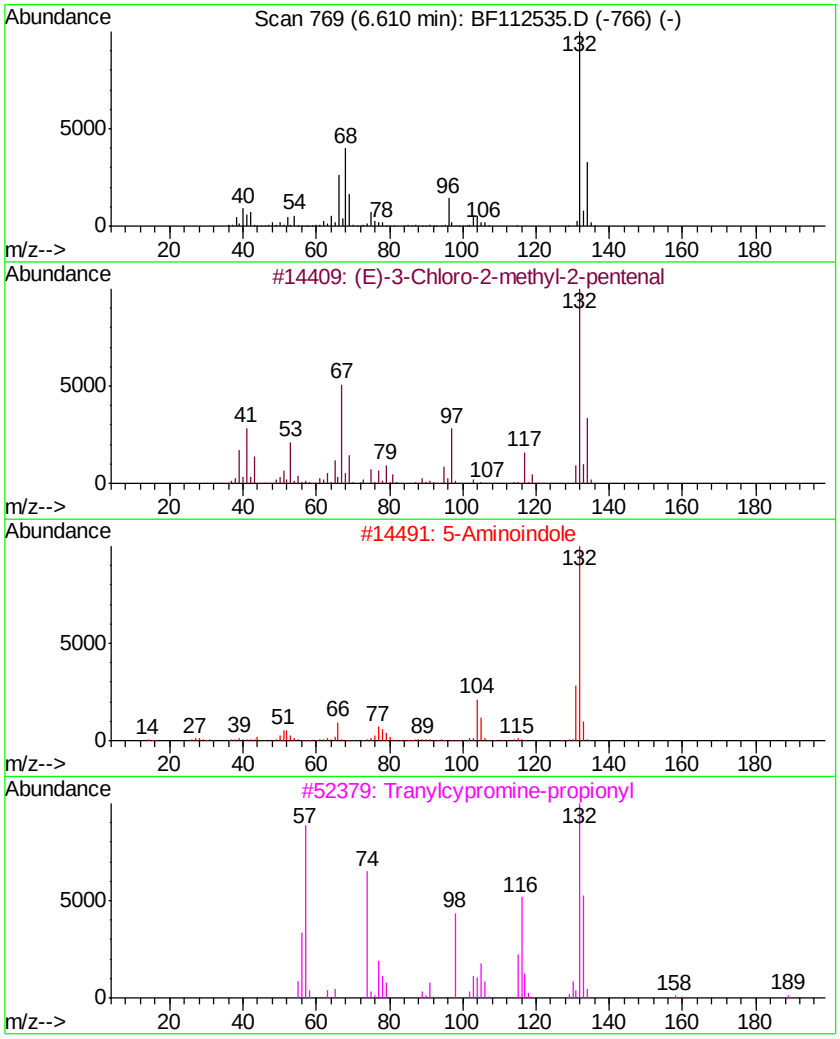
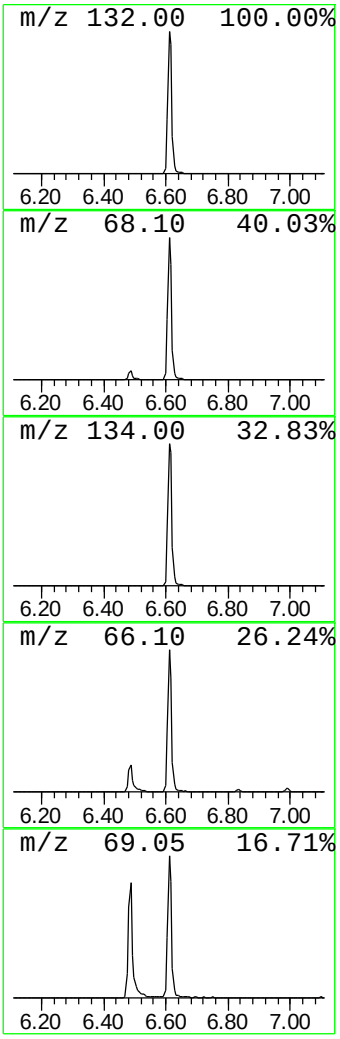
Peak Number 2 unknown6.61 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.61	64.86 ng	1797750	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	16
2	5-Aminoindole	132	C8H8N2	005192-03-0	12
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
4	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5	Benzene, 1-ethenyl-3,5-dimethyl-	132	C10H12	005379-20-4	9





Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF021319\
Data File : BF112535.D
Acq On : 13 Feb 2019 13:28
Operator : JU/SJ
Sample : K1442-06
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : COMP-12

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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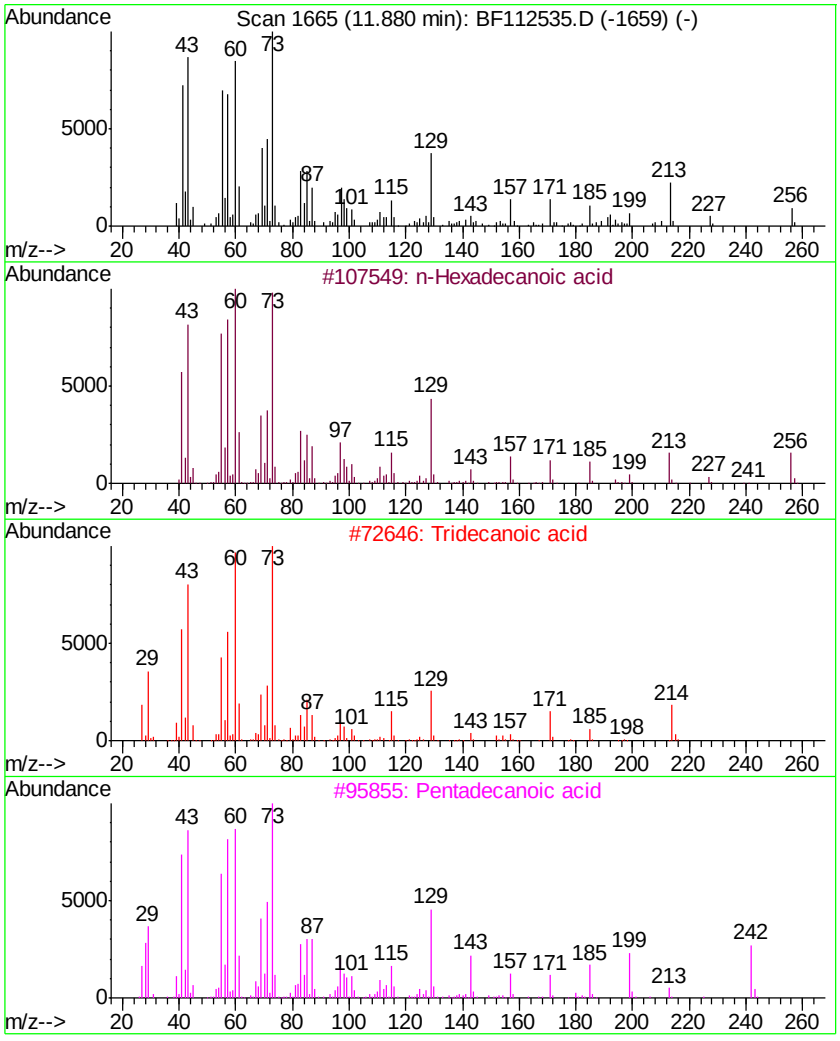
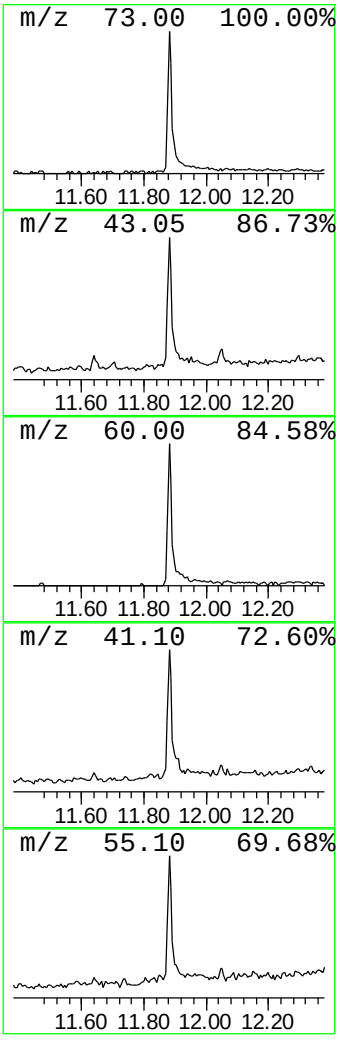
Peak Number 4 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.88	12.43 ng	412354	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	89
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	83
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	76
5	n-Decanoic acid	172	C10H20O2	000334-48-5	46





Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF021319\
Data File : BF112535.D
Acq On : 13 Feb 2019 13:28
Operator : JU/SJ
Sample : K1442-06
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : COMP-12

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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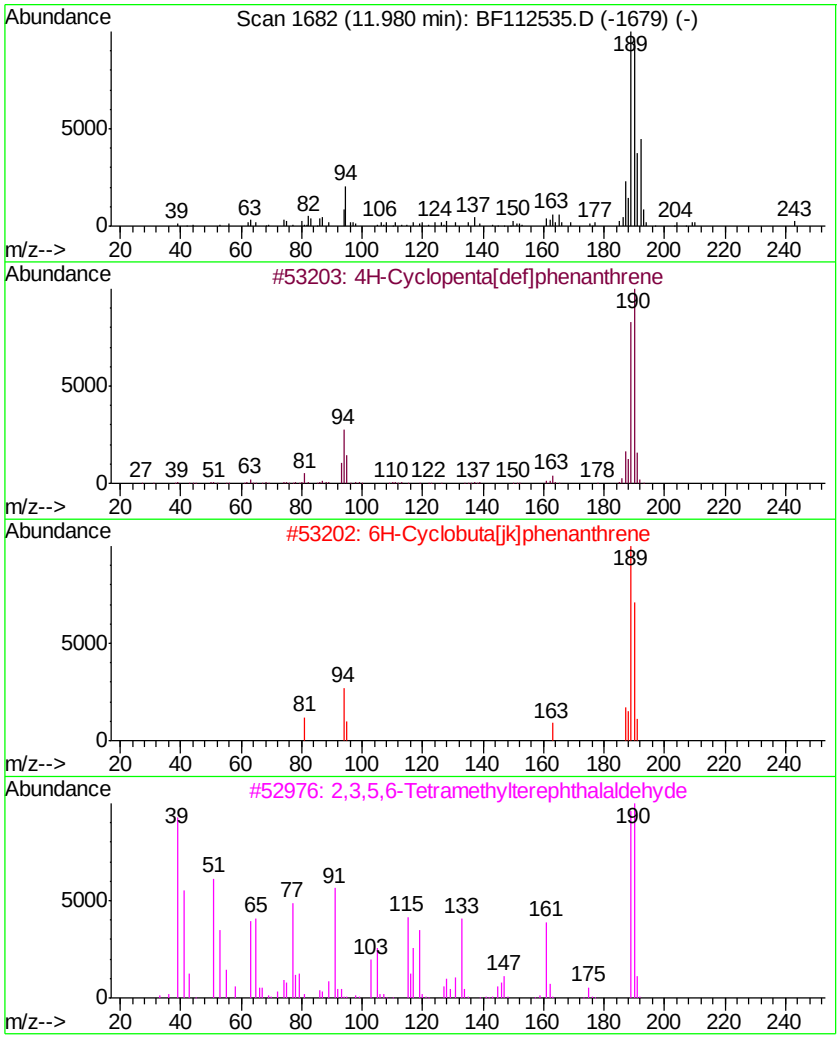
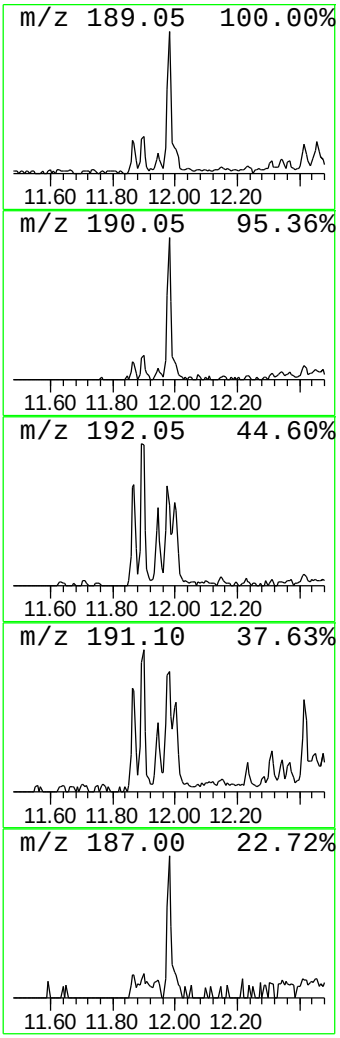
Peak Number 5 4H-Cyclopenta[def]phenanthrene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.98	2.53 ng	83761	Phenanthrene-d10	11.36

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	74
2	6H-Cyclobuta[jk]phenanthrene	190	C15H10	083469-43-6	59
3	2,3,5,6-Tetramethylterephthalald...	190	C12H14O2	007072-01-7	47
4	2,2'-Bis(4,5-dimethylimidazole)	190	C10H14N4	069286-06-2	36
5	Carbonic acid, ethyl 2-formyl-4,...	262	C10H8Cl2O4	1000331-34-4	33





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Misc :
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Instrument : BNA_F
ClientSampleId : COMP-12

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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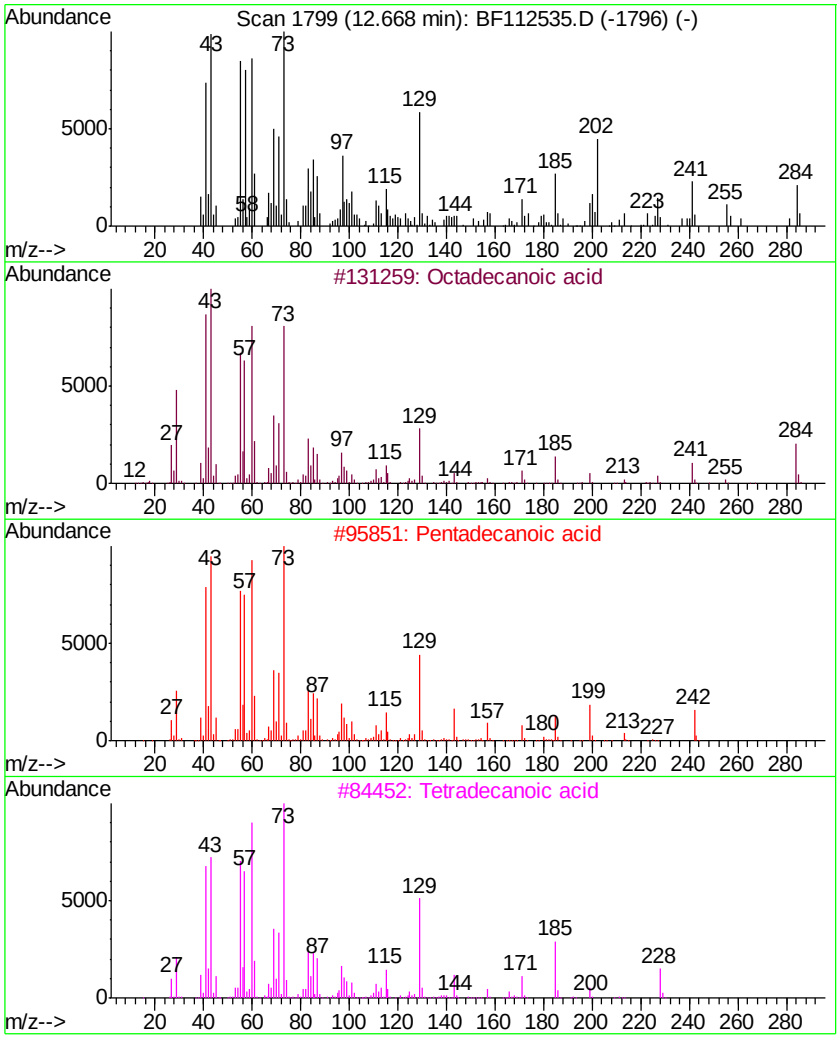
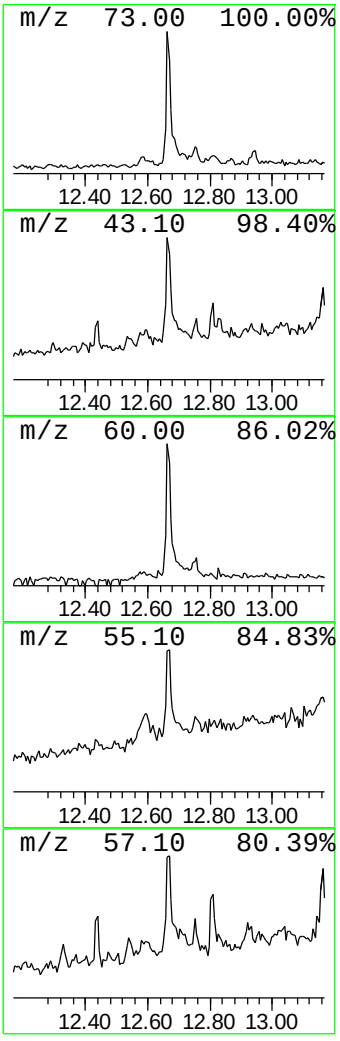
Peak Number 6 Octadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.67	5.07 ng	168284	Phenanthrene-d10	11.36

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	97
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	86
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	86
4	Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	64
5	Dodecanoic acid	200	C12H24O2	000143-07-7	60





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Data File : BF112535.D
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Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : COMP-12

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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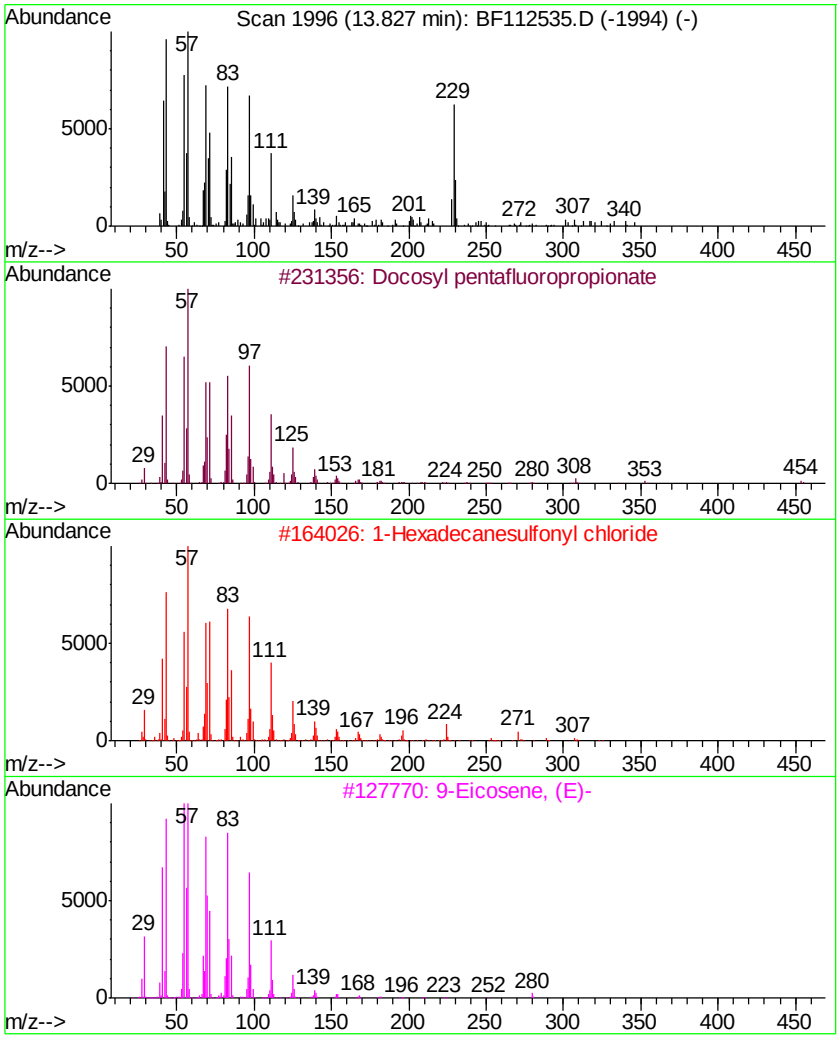
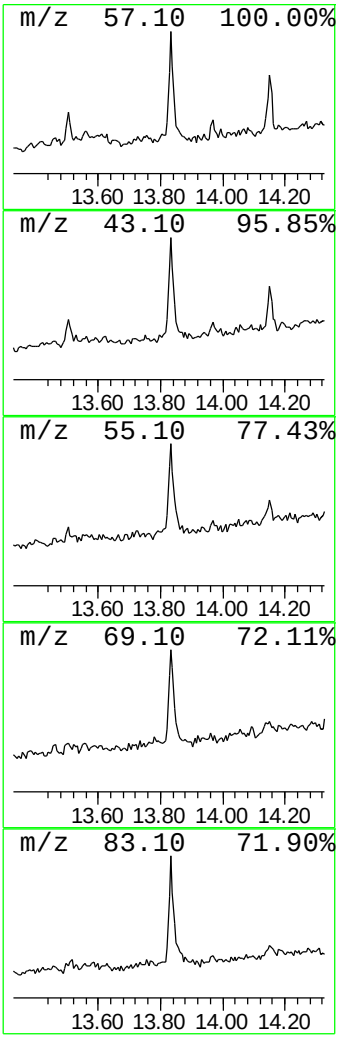
Peak Number 7 Docosyl pentafluoropropionate Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.83	4.49 ng	232645	Chrysene-d12	14.02

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Docosyl pentafluoropropionate	472	C25H45F5O2	1000351-80-9	81
2	1-Hexadecanesulfonyl chloride	324	C16H33ClO2S	038775-38-1	81
3	9-Eicosene, (E)-	280	C20H40	074685-29-3	78
4	Heptacosyl pentafluoropropionate	542	C30H55F5O2	1000351-81-6	76
5	Octacosyl heptafluorobutyrate	606	C32H57F7O2	1000351-83-6	76





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Instrument : BNA_F
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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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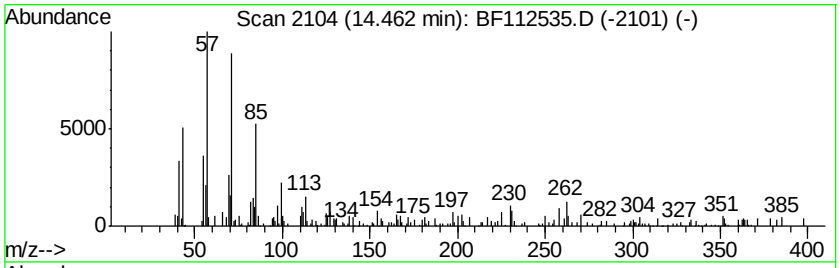
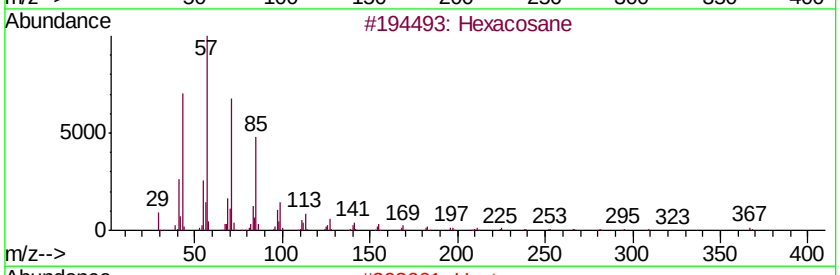
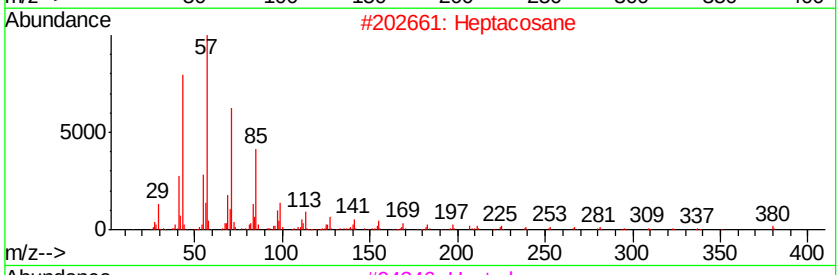
Peak Number 8 Hexacosane Concentration Rank 9

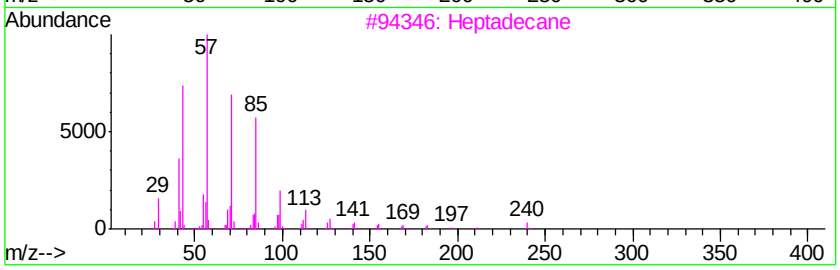
R.T.	EstConc	Area	Relative to ISTD	R.T.
14.46	2.19 ng	113797	Chrysene-d12	14.02

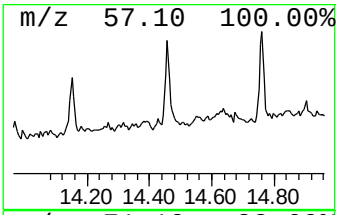
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosane	366	C26H54	000630-01-3	72
2	Heptacosane	380	C27H56	000593-49-7	72
3	Heptadecane	240	C17H36	000629-78-7	72
4	Tetradecane	198	C14H30	000629-59-4	70
5	Tridecane, 1-iodo-	310	C13H27I	035599-77-0	68

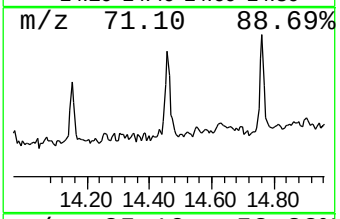


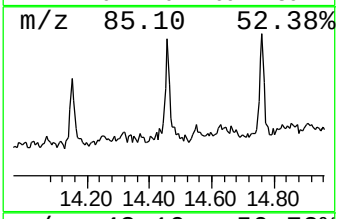


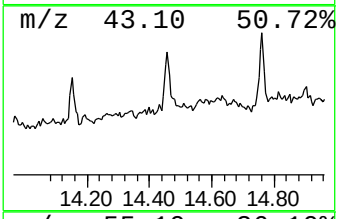


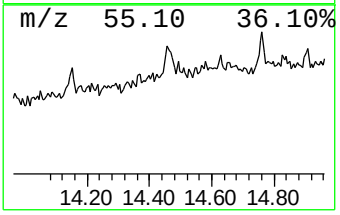












Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF021319\
Data File : BF112535.D
Acq On : 13 Feb 2019 13:28
Operator : JU/SJ
Sample : K1442-06
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : COMP-12

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

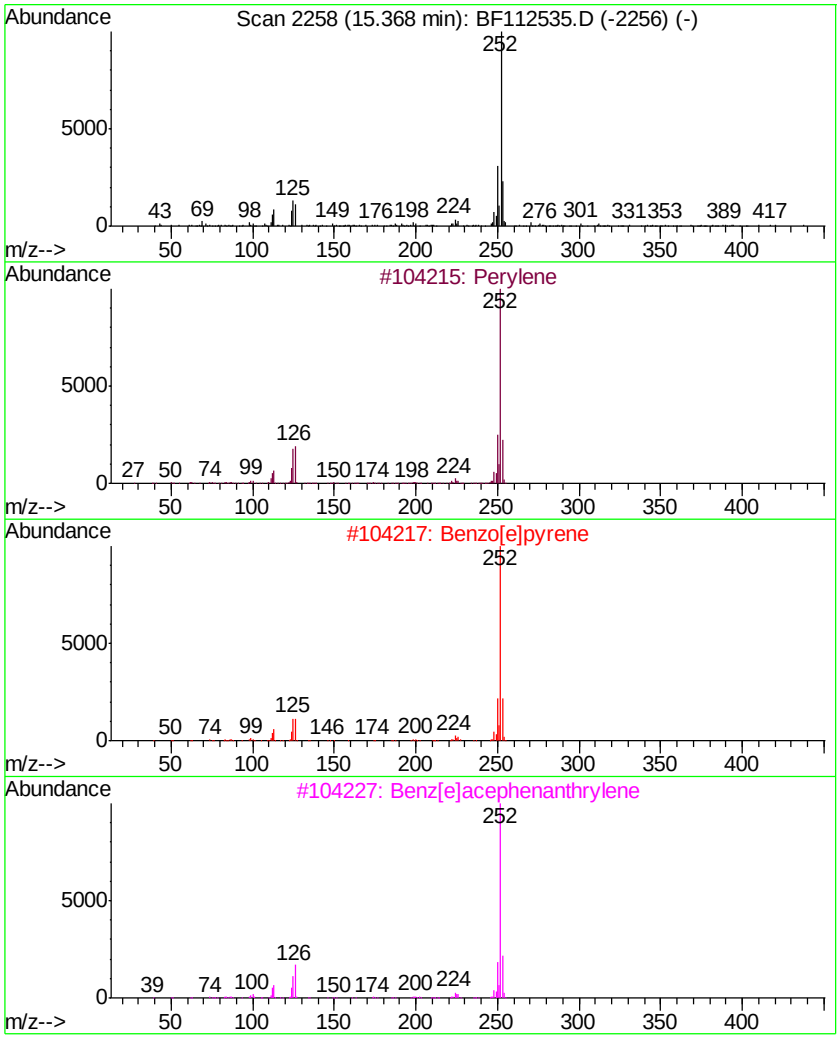
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

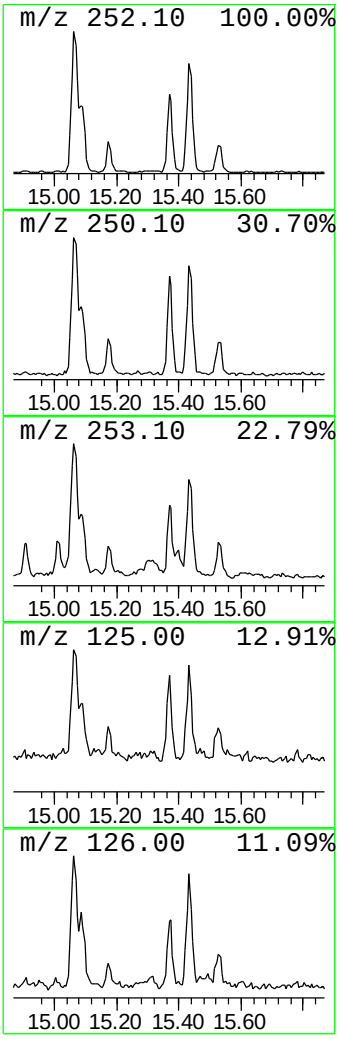
****

Peak Number 9 Perylene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.37	7.81 ng	160835	Perylene-d12	15.50

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Perylene	252	C20H12	000198-55-0	94
2	Benzo[e]pyrene	252	C20H12	000192-97-2	94
3	Benz[e]acephenanthrylene	252	C20H12	000205-99-2	90
4	Benzo[k]fluoranthene	252	C20H12	000207-08-9	89
5	Benzo[a]pyrene	252	C20H12	000050-32-8	81





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF021319\
Data File : BF112535.D
Acq On : 13 Feb 2019 13:28
Operator : JU/SJ
Sample : K1442-06
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : COMP-12

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	2.9	ng	79284	1	6.83	554371	20.0
unknown6.61	6.61	64.9	ng	1797750	1	6.83	554371	20.0
n-Hexadecanoic acid	11.88	12.4	ng	412354	4	11.36	663316	20.0
4H-Cyclopenta[def...	11.98	2.5	ng	83761	4	11.36	663316	20.0
Octadecanoic acid	12.67	5.1	ng	168284	4	11.36	663316	20.0
Docosyl pentafluo...	13.83	4.5	ng	232645	5	14.02	1037100	20.0
Hexacosane	14.46	2.2	ng	113797	5	14.02	1037100	20.0
Perylene	15.37	7.8	ng	160835	6	15.50	411912	20.0