LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF102419\
Data File : BF117516.D
Acq On : 24 Oct 2019 17:59
Operator : JU
Sample : K5499-03
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 194-84-(0-1)

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-BF101819.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	4.940	482	485	494	rBV	6654	10501	1.16%	0.102%
2	5.357	552	556	581	rBV	618458	783937	86.34%	7.621%
3	6.387	727	731	748	rBV	748438	873866	96.24%	8.496%
4	6.510	748	752	760	rVV	924896	908013	100.00%	8.828%
5	6.569	760	762	768	rVB4	7398	10435	1.15%	0.101%
6	6.734	787	790	801	rBV	235902	229288	25.25%	2.229%
7	6.887	812	816	832	rBV	751481	651329	71.73%	6.332%
8	7.298	882	886	902	rBV	526114	532430	58.64%	5.176%
9	8.010	1004	1007	1019	rBV	303199	302456	33.31%	2.940%
10	9.086	1186	1190	1201	rBV	1048269	869456	95.75%	8.453%
11	9.481	1254	1257	1265	rBV	143642	117913	12.99%	1.146%
12	9.763	1301	1305	1309	rBV	413664	336902	37.10%	3.275%
13	9.792	1309	1310	1317	rVB	17914	16522	1.82%	0.161%
14	10.316	1396	1399	1403	rBV	11790	13910	1.53%	0.135%
15	10.557	1436	1440	1453	rBV	469966	468021	51.54%	4.550%
16	10.669	1456	1459	1464	rVB3	8267	11502	1.27%	0.112%
17	11.110	1529	1534	1537	rBV4	10042	11953	1.32%	0.116%
18	11.145	1537	1540	1545	rVB2	12113	13028	1.43%	0.127%
19	11.251	1554	1558	1560	rBV	323778	293837	32.36%	2.857%
20	11.275	1560	1562	1569	rVV	214766	190568	20.99%	1.853%
21	11.328	1569	1571	1575	rVB	36250	30880	3.40%	0.300%
22	11.492	1595	1599	1605	rBV2	15446	24364	2.68%	0.237%
23	11.751	1641	1643	1645	rBV	27591	20986	2.31%	0.204%
24	11.780	1645	1648	1651	rVV	141226	137357	15.13%	1.335%
25	11.804	1651	1652	1655	rVV	31642	25135	2.77%	0.244%
26	11.863	1659	1662	1665	rVV2	42616	49424	5.44%	0.480%
27	11.886	1665	1666	1674	rVB2	18295	17171	1.89%	0.167%
28	12.045	1691	1693	1696	rVB	16479	14050	1.55%	0.137%
29	12.092	1698	1701	1704	rBV3	11421	11827	1.30%	0.115%
30	12.304	1734	1737	1740	rBV	18288	18520	2.04%	0.180%
31	12.333	1740	1742	1745	rVB3	20999	20179	2.22%	0.196%
32	12.398	1751	1753	1756	rVB2	10250	10513	1.16%	0.102%
33	12.463	1761	1764	1771	rBV	310097	297016	32.71%	2.888%
34	12.563	1778	1781	1787	rBV3	42524	55280	6.09%	0.537%

LSC Area Percent Report

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Acq On : 24 Oct 2019 17:59
Operator : JU
Sample : K5499-03
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 194-84-(0-1)

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-BF101819.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	12.616	1787	1790	1793	rVV3	17469	17528	1.93%	0.170%
36	12.692	1797	1803	1809	rVV	264784	287234	31.63%	2.792%
37	12.745	1810	1812	1816	rVB5	14047	16480	1.81%	0.160%
38	12.833	1822	1827	1830	rBV	578944	552002	60.79%	5.367%
39	12.916	1837	1841	1845	rBV3	13626	20298	2.24%	0.197%
40	13.004	1852	1856	1857	rBV4	15993	19182	2.11%	0.186%
41	13.022	1857	1859	1862	rVV	27558	26090	2.87%	0.254%
42	13.063	1863	1866	1868	rVV	26747	25726	2.83%	0.250%
43	13.092	1868	1871	1874	rVV	14258	15930	1.75%	0.155%
44	13.127	1874	1877	1879	rBV2	18531	18440	2.03%	0.179%
45	13.222	1891	1893	1896	rBV2	11602	11330	1.25%	0.110%
46	13.251	1896	1898	1901	rVV3	13115	13015	1.43%	0.127%
47	13.298	1904	1906	1910	rVB	37658	37054	4.08%	0.360%
48	13.545	1945	1948	1951	rVB3	23869	26174	2.88%	0.254%
49	13.645	1962	1965	1967	rBV2	26118	30566	3.37%	0.297%
50	13.733	1977	1980	1989	rVB2	93933	161416	17.78%	1.569%
51	13.863	1998	2002	2004	rBV	240443	226023	24.89%	2.197%
52	13.892	2004	2007	2010	rVV2	302749	371038	40.86%	3.607%
53	13.921	2010	2012	2015	rVB	115212	104104	11.47%	1.012%
54	13.998	2023	2025	2028	rVB2	16002	13199	1.45%	0.128%
55	14.351	2083	2085	2087	rBV2	33769	31049	3.42%	0.302%
56	14.716	2145	2147	2152	rVB	37712	43932	4.84%	0.427%
57	14.921	2179	2182	2185	rBV	113095	148460	16.35%	1.443%
58	15.210	2228	2231	2236	rVB	77280	79611	8.77%	0.774%
59	15.274	2238	2242	2246	rVB	92873	107776	11.87%	1.048%
60	15.327	2247	2251	2255	rBV	191666	256978	28.30%	2.498%
61	15.727	2315	2319	2325	rVB	54918	78511	8.65%	0.763%
62	16.745	2488	2492	2499	rVB2	60442	112577	12.40%	1.094%
63	17.168	2560	2564	2571	rVB2	24390	55672	6.13%	0.541%

Sum of corrected areas: 10285964

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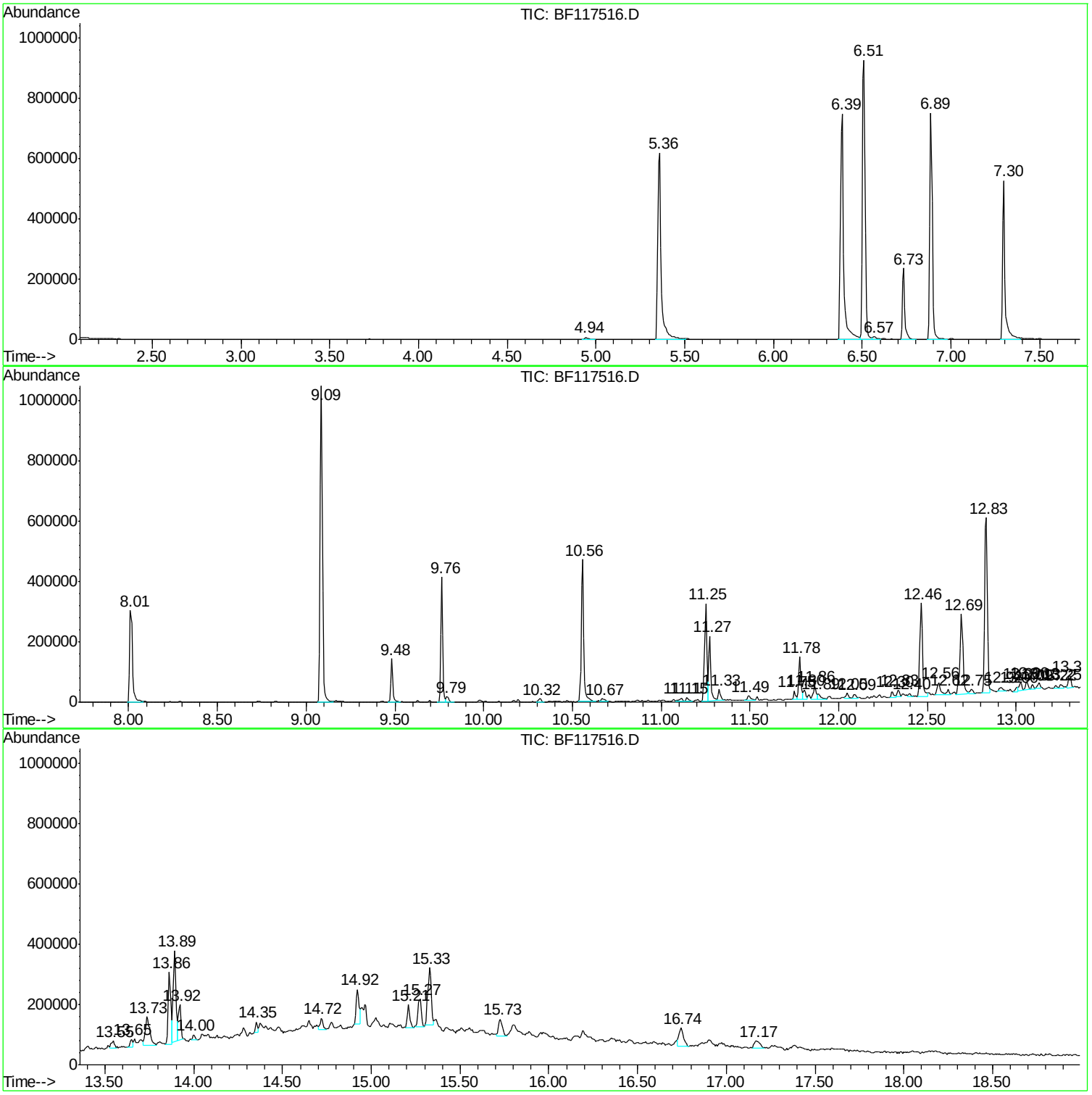
Instrument :
BNA_F
ClientSampleId :
194-84-(0-1)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101819.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

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Instrument : BNA_F
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TIC Library : C:\DATABASE\NIST11.L
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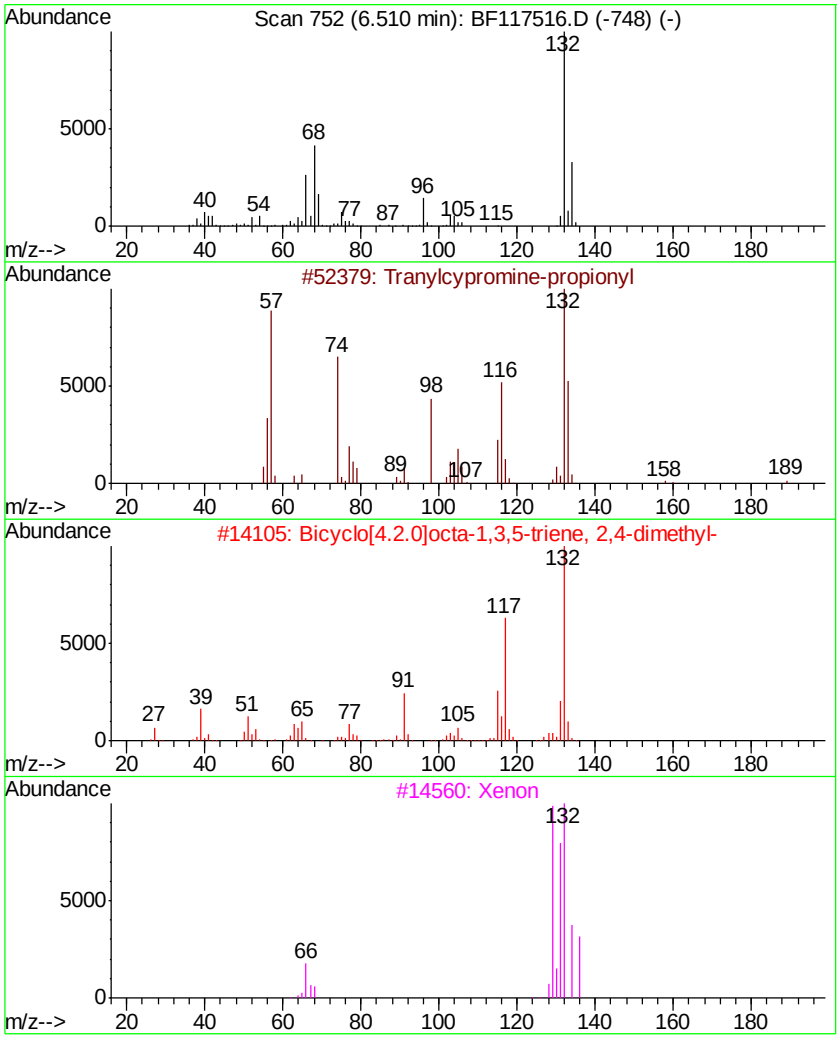
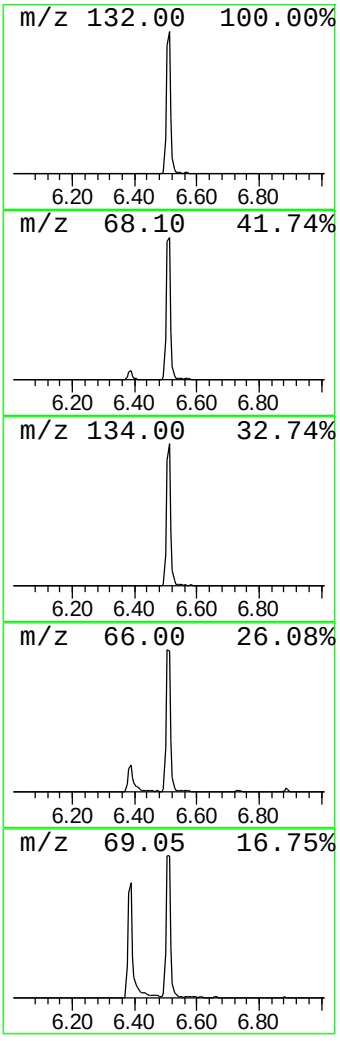
Peak Number 1 unknown6.51 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.51	79.20 ng	908013	1,4-Dichlorobenzene-d4	6.73

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
2	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
3	Xenon	132	Xe	007440-63-3	9
4	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9
5	1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9





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Acq On : 24 Oct 2019 17:59
Operator : JU
Sample : K5499-03
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 194-84-(0-1)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101819.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
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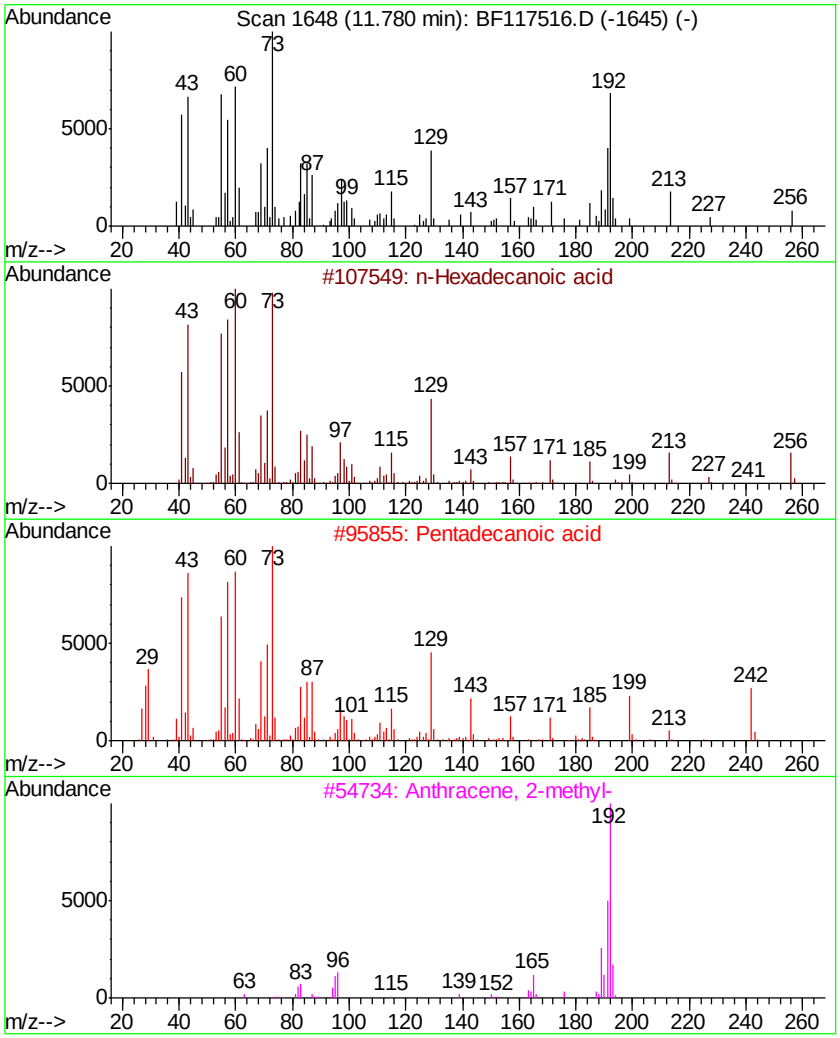
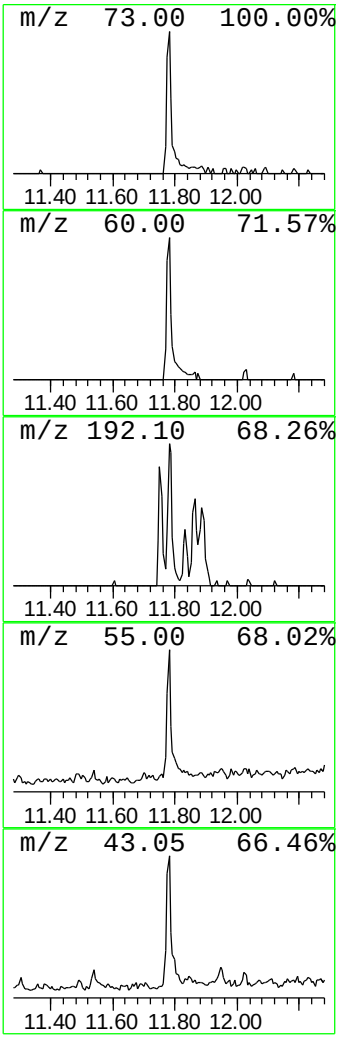
Peak Number 3 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.78	9.35 ng	137357	Phenanthrene-d10	11.25

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	92
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	70
3	Anthracene, 2-methyl-	192	C15H12	000613-12-7	68
4	Anthracene, 9-methyl-	192	C15H12	000779-02-2	56
5	Phenanthrene, 3-methyl-	192	C15H12	000832-71-3	56





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Sample : K5499-03
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 194-84-(0-1)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101819.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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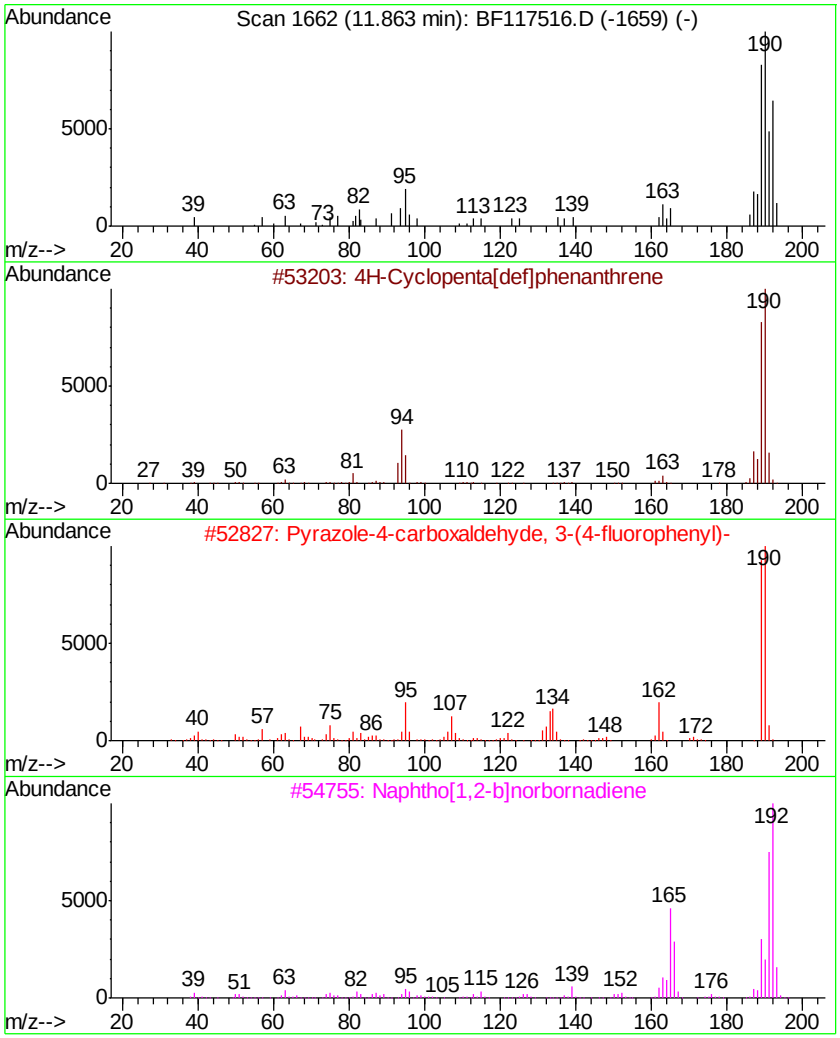
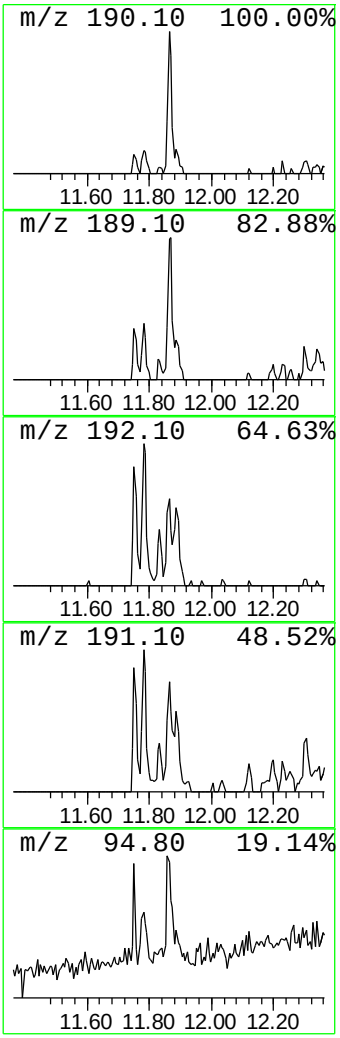
Peak Number 4 4H-Cyclopenta[def]phenanthrene Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.86	3.36 ng	49424	Phenanthrene-d10	11.25

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	58
2	Pyrazole-4-carboxaldehyde, 3-(4-...	190	C10H7FN2O	306936-57-2	49
3	Naphtho[1,2-b]norbornadiene	192	C15H12	1000210-14-8	30
4	Phenanthrene, 4-methyl-	192	C15H12	000832-64-4	30
5	5-Thiazolecarboxamide, 4-amino-2...	189	C5H7N3OS2	1000338-08-9	27





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Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 194-84-(0-1)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101819.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
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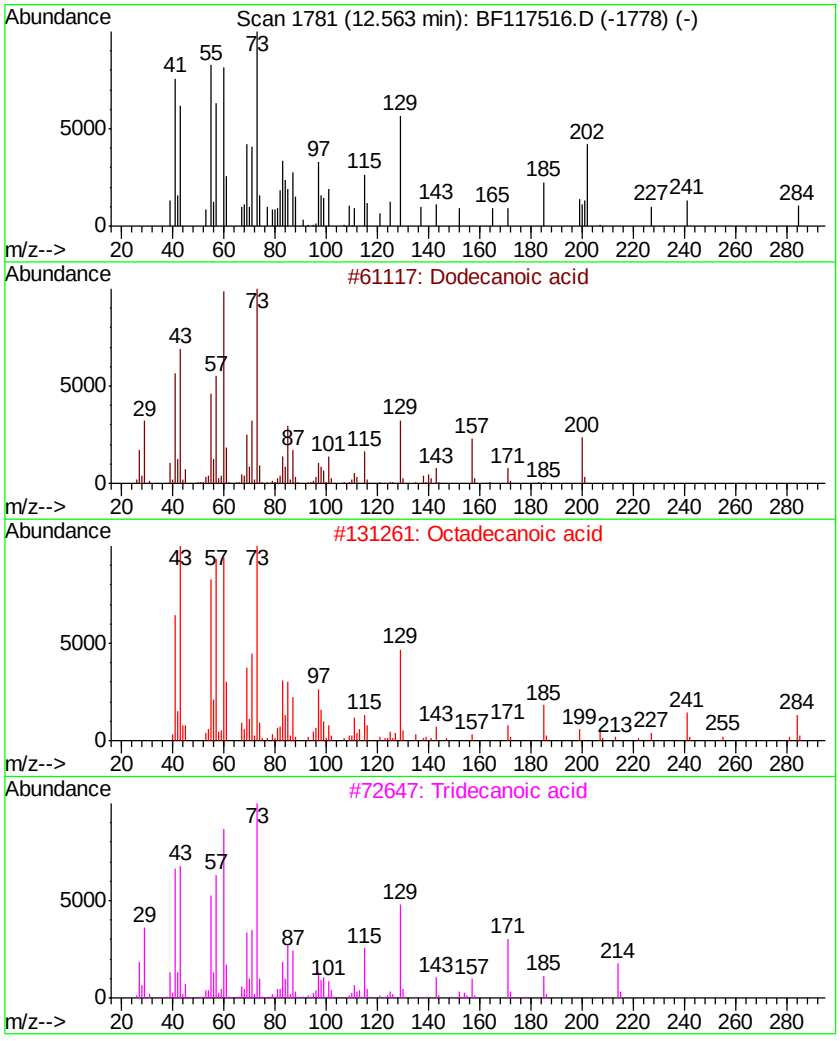
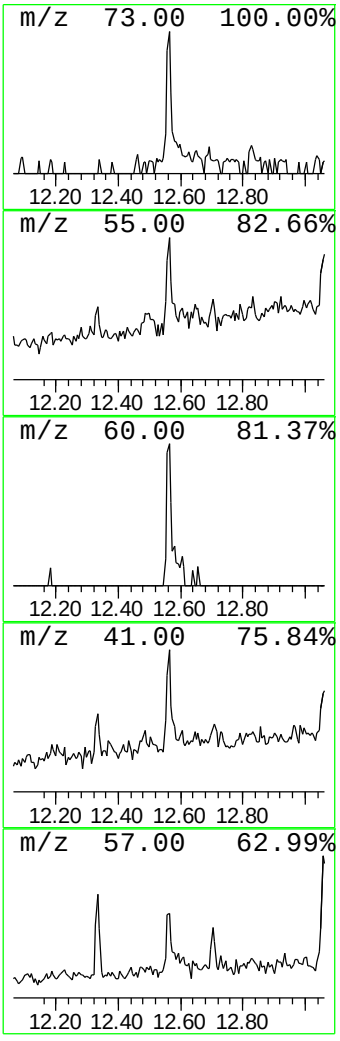
Peak Number 5 Dodecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.56	3.76 ng	55280	Phenanthrene-d10	11.25

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dodecanoic acid	200	C12H24O2	000143-07-7	64
2	Octadecanoic acid	284	C18H36O2	000057-11-4	50
3	Tridecanoic acid	214	C13H26O2	000638-53-9	50
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	47
5	Undecanoic acid	186	C11H22O2	000112-37-8	47





Library Search Compound Report

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Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 194-84-(0-1)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101819.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
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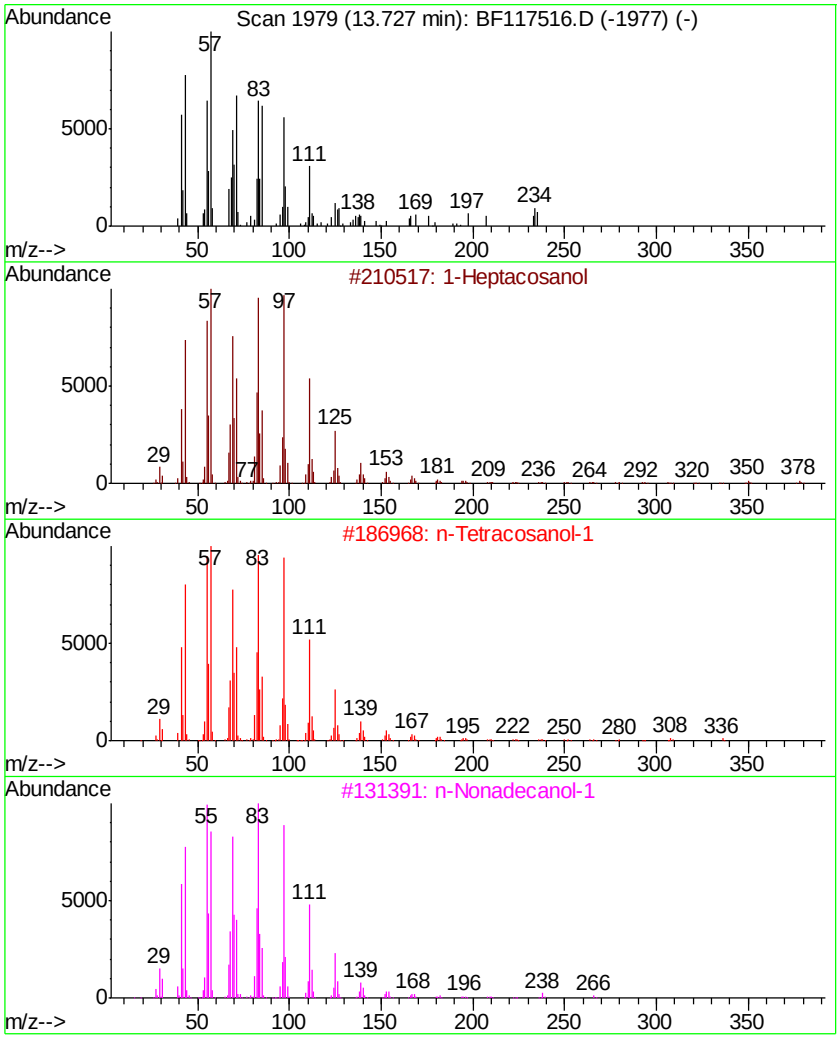
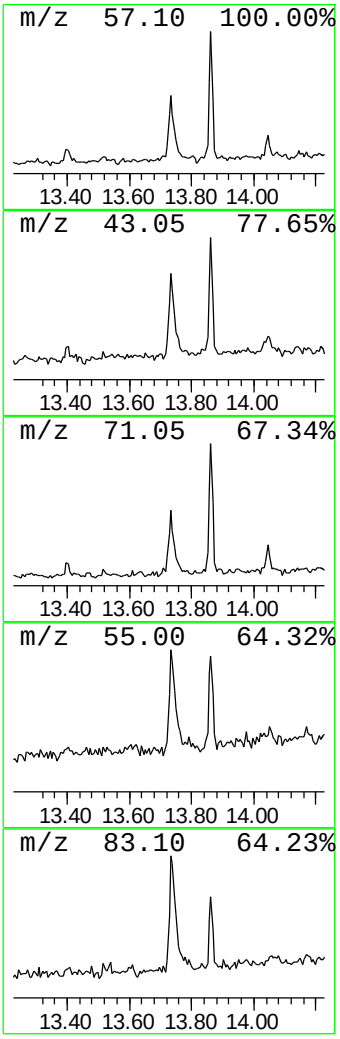
Peak Number 6 1-Heptacosanol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.73	8.70 ng	161416	Chrysene-d12	13.89

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heptacosanol	396	C27H56O	002004-39-9	76
2	n-Tetracosanol-1	354	C24H50O	000506-51-4	76
3	n-Nonadecanol-1	284	C19H40O	001454-84-8	70
4	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	64
5	Tricosyl heptafluorobutyrate	536	C27H47F7O2	1000351-83-4	64





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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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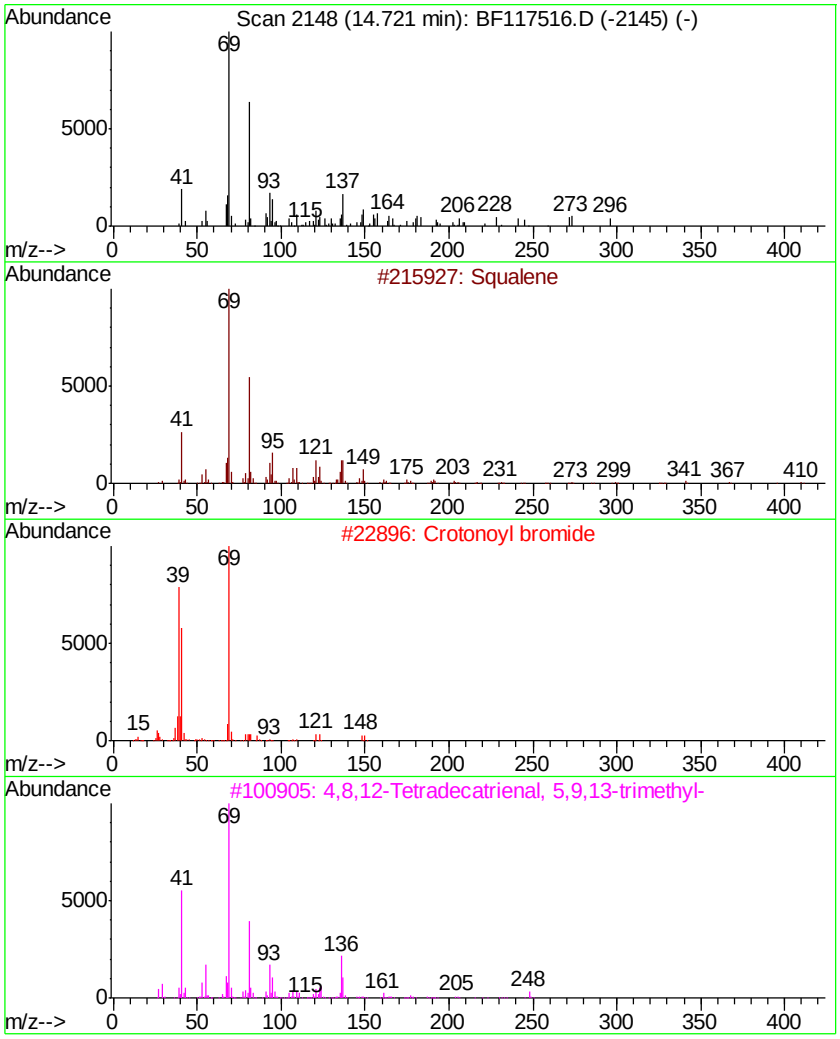
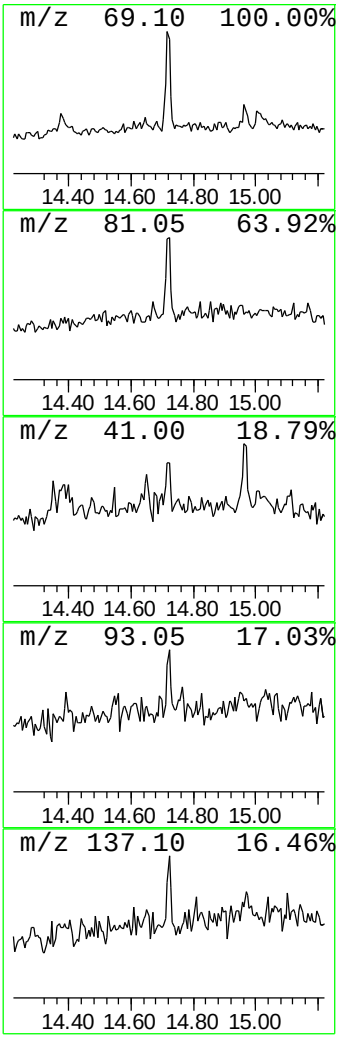
Peak Number 7 Squalene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.72	3.42 ng	43932	Perylene-d12	15.33

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Squalene	410	C30H50	000111-02-4	59
2	Crotonoyl bromide	148	C4H5BrO	055600-70-9	49
3	4,8,12-Tetradecatrienal, 5,9,13-...	248	C17H28O	066408-55-7	45
4	6,11-Dimethyl-2,6,10-dodecatrien...	208	C14H24O	1000196-53-3	42
5	2,6,10-Dodecatrienal, 3,7,11-tri...	220	C15H24O	004380-32-9	42





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Sample : K5499-03
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 194-84-(0-1)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101819.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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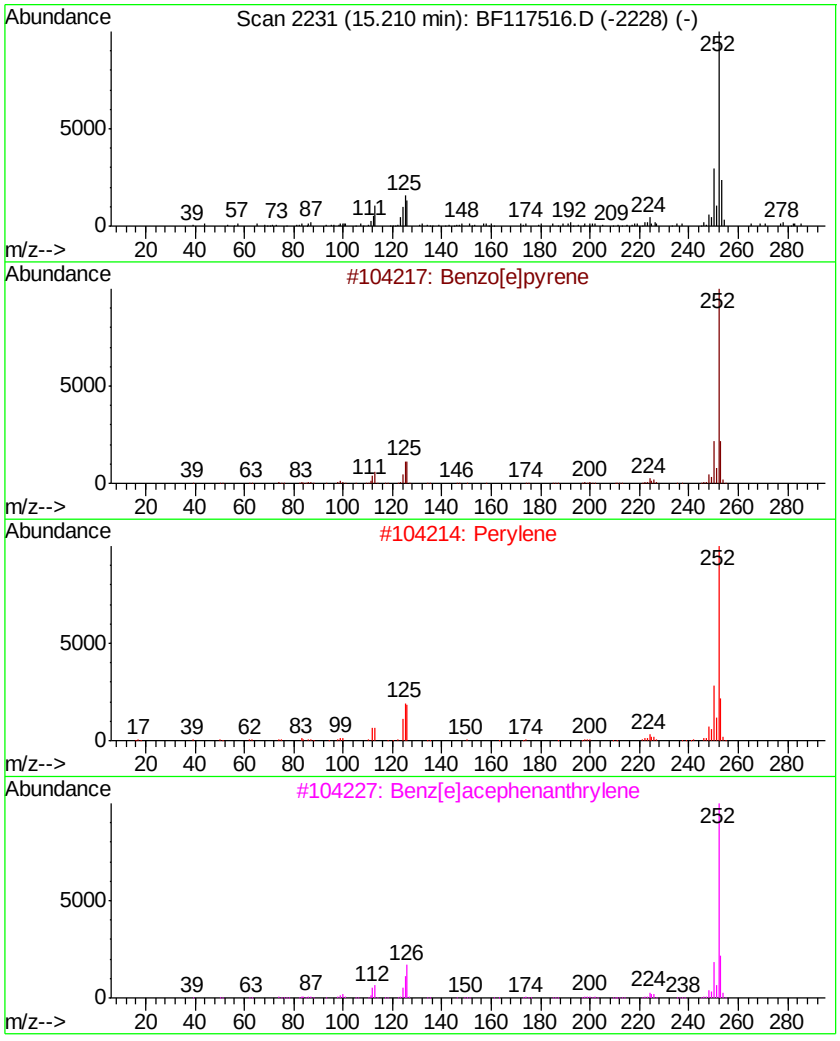
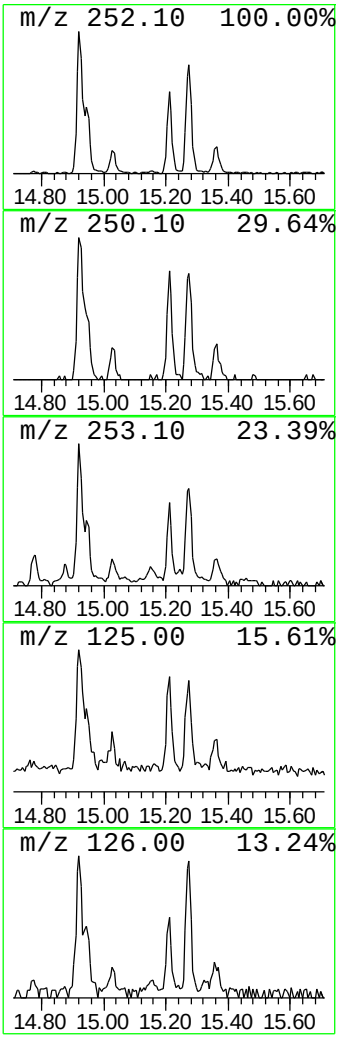
Peak Number 8 Perylene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.21	6.20 ng	79611	Perylene-d12	15.33

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[e]pyrene	252	C20H12	000192-97-2	95
2	Perylene	252	C20H12	000198-55-0	93
3	Benz[e]acephenanthrylene	252	C20H12	000205-99-2	90
4	Benzo[k]fluoranthene	252	C20H12	000207-08-9	90
5	Benzo[a]pyrene	252	C20H12	000050-32-8	87





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Instrument : BNA_F
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101819.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

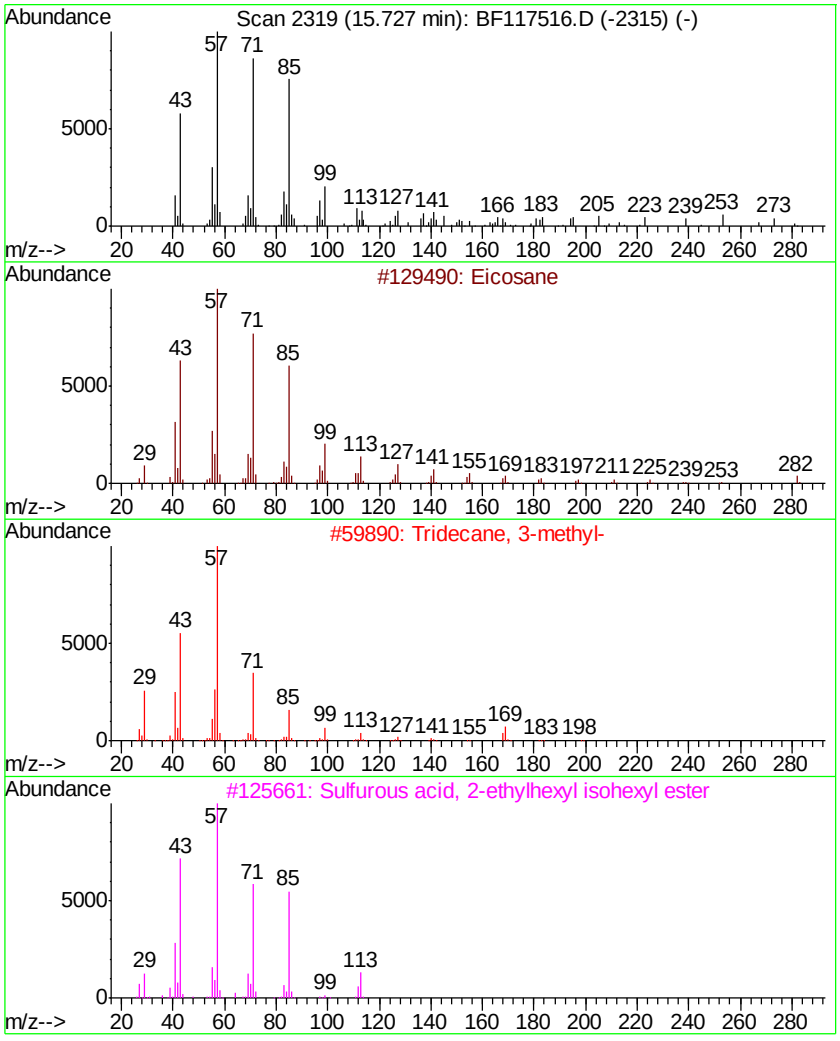
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

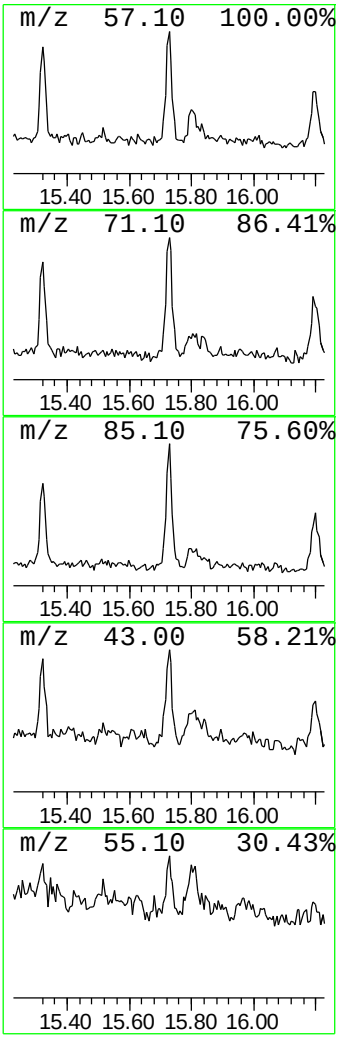
****

Peak Number 9 Tridecane, 3-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.73	6.11 ng	78511	Perylene-d12	15.33

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	83
2	Tridecane, 3-methyl-	198	C14H30	006418-41-3	72
3	Sulfurous acid, 2-ethylhexyl iso...	278	C14H30O3S	1000309-19-0	59
4	Pentacosane	352	C25H52	000629-99-2	59
5	Nonadecane, 4-methyl-	282	C20H42	025117-27-5	49





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF102419\
Data File : BF117516.D
Acq On : 24 Oct 2019 17:59
Operator : JU
Sample : K5499-03
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 194-84-(0-1)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101819.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
unknown6.51	6.51	79.2	ng	908013	1	6.73	229288	20.0
n-Hexadecanoic acid	11.78	9.3	ng	137357	4	11.25	293837	20.0
4H-Cyclopenta[def...	11.86	3.4	ng	49424	4	11.25	293837	20.0
Dodecanoic acid	12.56	3.8	ng	55280	4	11.25	293837	20.0
1-Heptacosanol	13.73	8.7	ng	161416	5	13.89	371038	20.0
Squalene	14.72	3.4	ng	43932	6	15.33	256978	20.0
Perylene	15.21	6.2	ng	79611	6	15.33	256978	20.0
Tridecane, 3-methyl-	15.73	6.1	ng	78511	6	15.33	256978	20.0