LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF112119\
Data File : BF117909.D
Acq On : 21 Nov 2019 13:53
Operator : JU
Sample : K5932-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RBR200027-1A-415

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-BF111319.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	2.169	9	14	31	rVB	665963	956049	21.59%	1.877%
2	5.122	511	516	526	rVB	431798	499145	11.27%	0.980%
3	5.528	580	585	588	rBV	3002868	2673654	60.39%	5.249%
4	6.539	751	757	768	rBV	2756173	2923100	66.02%	5.739%
5	6.681	777	781	785	rBV	3371359	3002111	67.81%	5.894%
6	6.916	817	821	824	rBV	1048629	793142	17.91%	1.557%
7	7.075	844	848	851	rBV	2720943	2320205	52.41%	4.555%
8	7.475	912	916	919	rBV	2102019	2021302	45.66%	3.969%
9	8.204	1036	1040	1043	rBV	1441459	1212359	27.38%	2.380%
10	9.280	1219	1223	1226	rBV	4732704	3987765	90.07%	7.829%
11	9.675	1286	1290	1295	rBV	810106	663511	14.99%	1.303%
12	9.963	1336	1339	1343	rBV	1642763	1513329	34.18%	2.971%
13	10.757	1469	1474	1477	rBV	2836645	2621653	59.22%	5.147%
14	11.457	1589	1593	1595	rBV	2064903	1664785	37.60%	3.269%
15	11.480	1595	1597	1601	rVV	824010	637521	14.40%	1.252%
16	11.533	1601	1606	1609	rVB	124260	144826	3.27%	0.284%
17	11.686	1626	1632	1640	rBV2	109880	163835	3.70%	0.322%
18	11.980	1673	1682	1689	rBV2	671856	836783	18.90%	1.643%
19	12.074	1694	1698	1700	rVV2	188291	203743	4.60%	0.400%
20	12.092	1700	1701	1705	rVB	68443	49765	1.12%	0.098%
21	12.257	1726	1729	1731	rBV	66515	56115	1.27%	0.110%
22	12.280	1731	1733	1736	rVB	83712	69269	1.56%	0.136%
23	12.510	1768	1772	1775	rBV2	134813	169798	3.84%	0.333%
24	12.545	1775	1778	1781	rVV3	65303	99091	2.24%	0.195%
25	12.592	1784	1786	1791	rVB	77815	82946	1.87%	0.163%
26	12.674	1796	1800	1803	rBV	1806785	1526514	34.48%	2.997%
27	12.768	1812	1816	1824	rBV	949930	1027225	23.20%	2.017%
28	12.827	1824	1826	1829	rVV	77143	89761	2.03%	0.176%
29	12.904	1833	1839	1845	rVV	1556848	1575775	35.59%	3.094%
30	12.951	1845	1847	1851	rVB2	62425	64301	1.45%	0.126%
31	13.045	1859	1863	1870	rVB	4445405	4427336	100.00%	8.692%
32	13.121	1871	1876	1879	rBV3	90907	147208	3.32%	0.289%
33	13.210	1887	1891	1892	rBV3	82002	91585	2.07%	0.180%
34	13.233	1892	1895	1898	rVB	233708	213300	4.82%	0.419%

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Misc :
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Instrument : BNA_F
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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

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Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF111319.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	13.268	1898	1901	1903	rBV2	68247	76075	1.72%	0.149%
36	13.298	1903	1906	1909	rVB	157497	118157	2.67%	0.232%
37	13.333	1909	1912	1915	rBV2	138229	142478	3.22%	0.280%
38	13.427	1925	1928	1931	rVB	84089	82598	1.87%	0.162%
39	13.463	1931	1934	1937	rBV2	89618	103582	2.34%	0.203%
40	13.615	1956	1960	1962	rBV4	48020	71421	1.61%	0.140%
41	13.739	1978	1981	1986	rVB	122647	125681	2.84%	0.247%
42	13.857	1995	2001	2003	rBV3	145537	225562	5.09%	0.443%
43	13.880	2003	2005	2007	rVV	133755	120015	2.71%	0.236%
44	13.904	2007	2009	2013	rVV2	122205	171208	3.87%	0.336%
45	13.951	2013	2017	2026	rVB5	290916	519647	11.74%	1.020%
46	14.104	2035	2043	2046	rBV2	1742675	2519834	56.92%	4.947%
47	14.133	2046	2048	2053	rVB	718678	634682	14.34%	1.246%
48	14.210	2059	2061	2065	rVB	124797	103439	2.34%	0.203%
49	14.262	2065	2070	2073	rBV3	66117	109226	2.47%	0.214%
50	14.327	2077	2081	2085	rVB3	72042	106893	2.41%	0.210%
51	14.492	2104	2109	2112	rVB	160732	170989	3.86%	0.336%
52	14.521	2112	2114	2118	rVB	91162	90867	2.05%	0.178%
53	14.568	2118	2122	2123	rBV3	100609	97661	2.21%	0.192%
54	14.615	2128	2130	2132	rVV	115936	105594	2.39%	0.207%
55	14.639	2132	2134	2139	rVB3	111215	107730	2.43%	0.212%
56	14.692	2139	2143	2146	rBV5	53640	68790	1.55%	0.135%
57	14.804	2159	2162	2165	rBV3	56672	87328	1.97%	0.171%
58	14.833	2165	2167	2172	rVB4	57444	76746	1.73%	0.151%
59	14.886	2173	2176	2180	rBV2	141495	143061	3.23%	0.281%
60	14.968	2186	2190	2193	rBV	159001	175679	3.97%	0.345%
61	15.168	2219	2224	2227	rBV	667224	1077599	24.34%	2.116%
62	15.239	2233	2236	2239	rVB2	139182	148826	3.36%	0.292%
63	15.274	2239	2242	2246	rVB	113442	124364	2.81%	0.244%
64	15.374	2255	2259	2260	rBV3	50188	68754	1.55%	0.135%
65	15.480	2273	2277	2283	rVB	399036	538965	12.17%	1.058%
66	15.545	2284	2288	2294	rVB	577174	700413	15.82%	1.375%
67	15.615	2295	2300	2303	rVV	1062950	1436989	32.46%	2.821%
68	15.645	2303	2305	2311	rVB3	277490	324932	7.34%	0.638%
69	16.104	2379	2383	2389	rVB2	96002	157950	3.57%	0.310%
70	16.204	2396	2400	2409	rVB6	60331	134404	3.04%	0.264%
71	16.633	2469	2473	2480	rBV5	56801	119608	2.70%	0.235%

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Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RBR200027-1A-415

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

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Peak separation: 5

Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF111319.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

72	17.145	2554	2560	2569	rVB2	282240	564112	12.74%	1.108%
73	17.327	2587	2591	2596	rBV2	55607	91243	2.06%	0.179%
74	17.609	2632	2639	2650	rVB	220822	470744	10.63%	0.924%
75	17.850	2676	2680	2686	rVB2	49227	90911	2.05%	0.178%

Sum of corrected areas: 50933564

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Operator : JU
Sample : K5932-01
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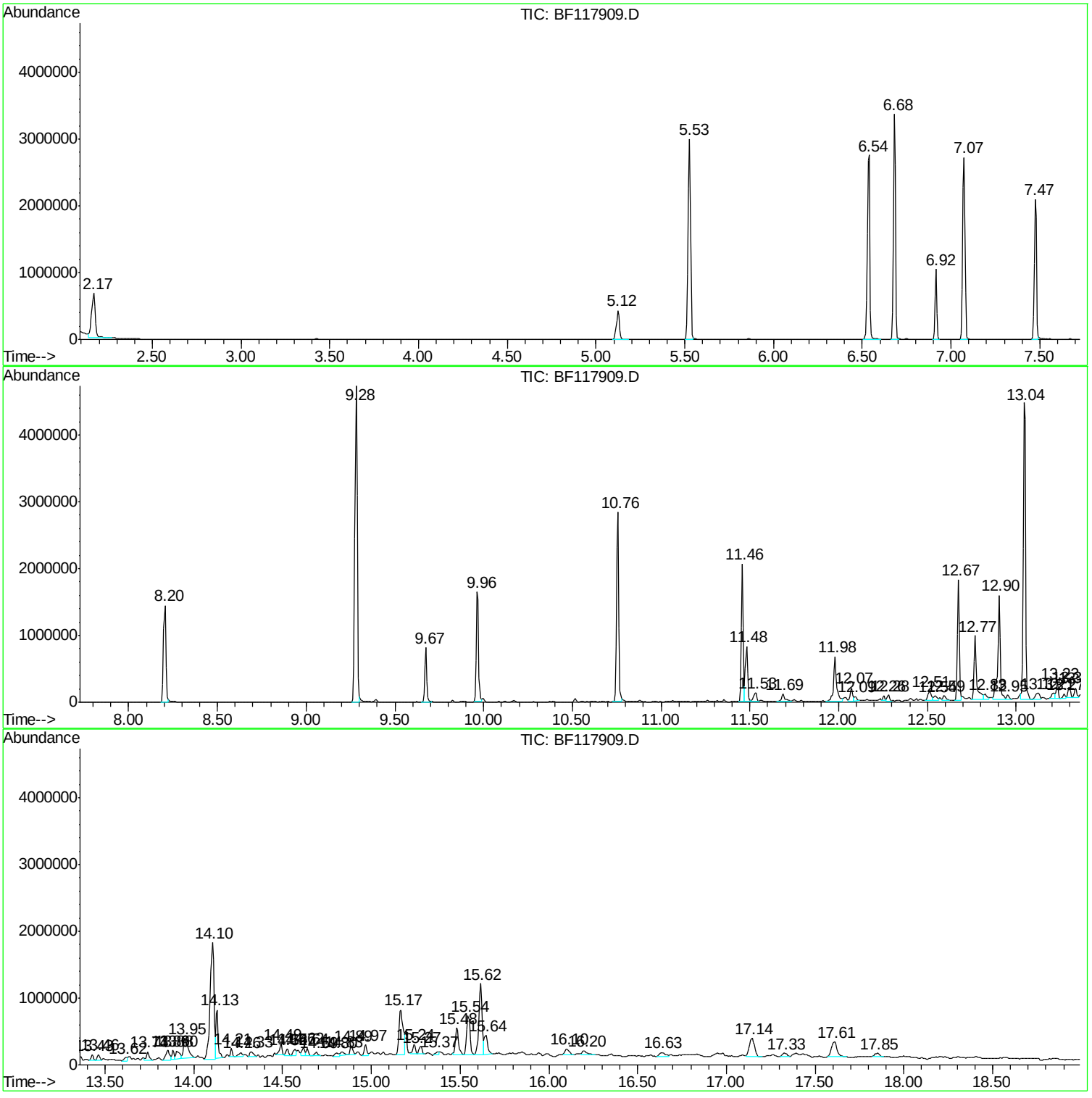
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RBR200027-1A-415

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF111319.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\BF112119\
Data File : BF117909.D
Acq On : 21 Nov 2019 13:53
Operator : JU
Sample : K5932-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF111319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

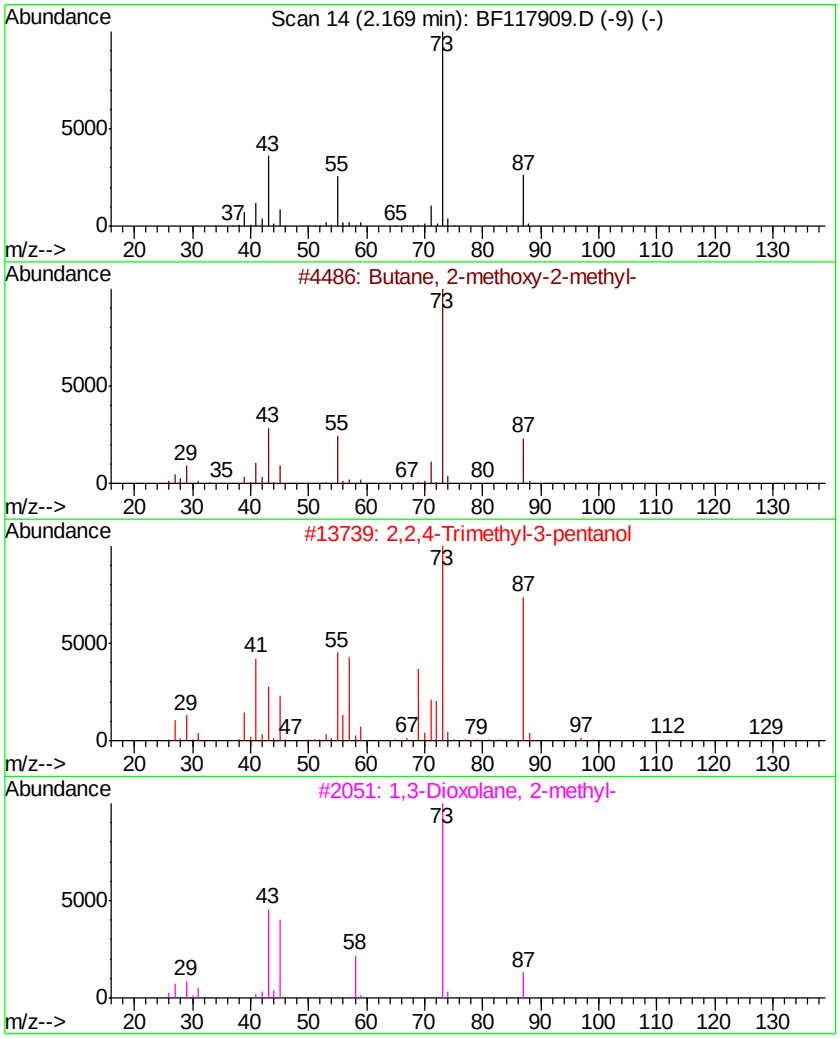
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

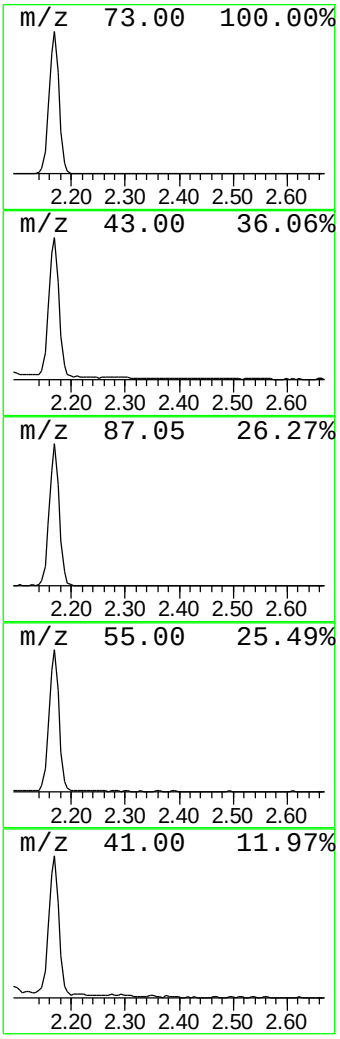
****

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.17	24.11 ng	956049	1,4-Dichlorobenzene-d4	6.92

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
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	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	23
5	Silane, tetramethyl-	88	C4H12Si	000075-76-3	17





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Operator : JU
Sample : K5932-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RBR200027-1A-415

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF111319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

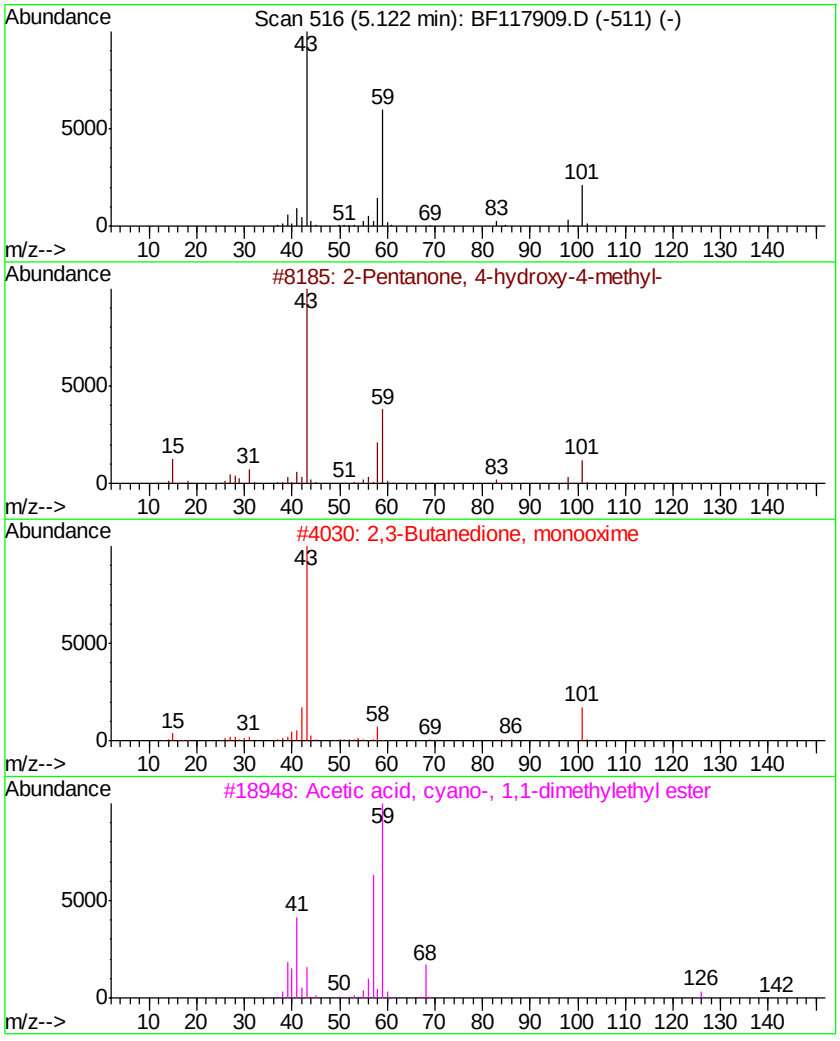
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

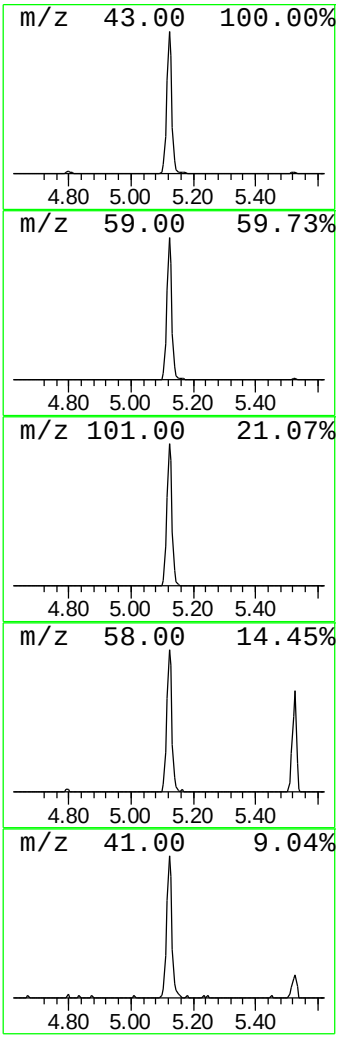
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.12	12.59 ng	499145	1,4-Dichlorobenzene-d4	6.92

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	35
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
4	5-Hexen-2-one	98	C6H10O	000109-49-9	9
5	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF112119\
Data File : BF117909.D
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Operator : JU
Sample : K5932-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RBR200027-1A-415

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF111319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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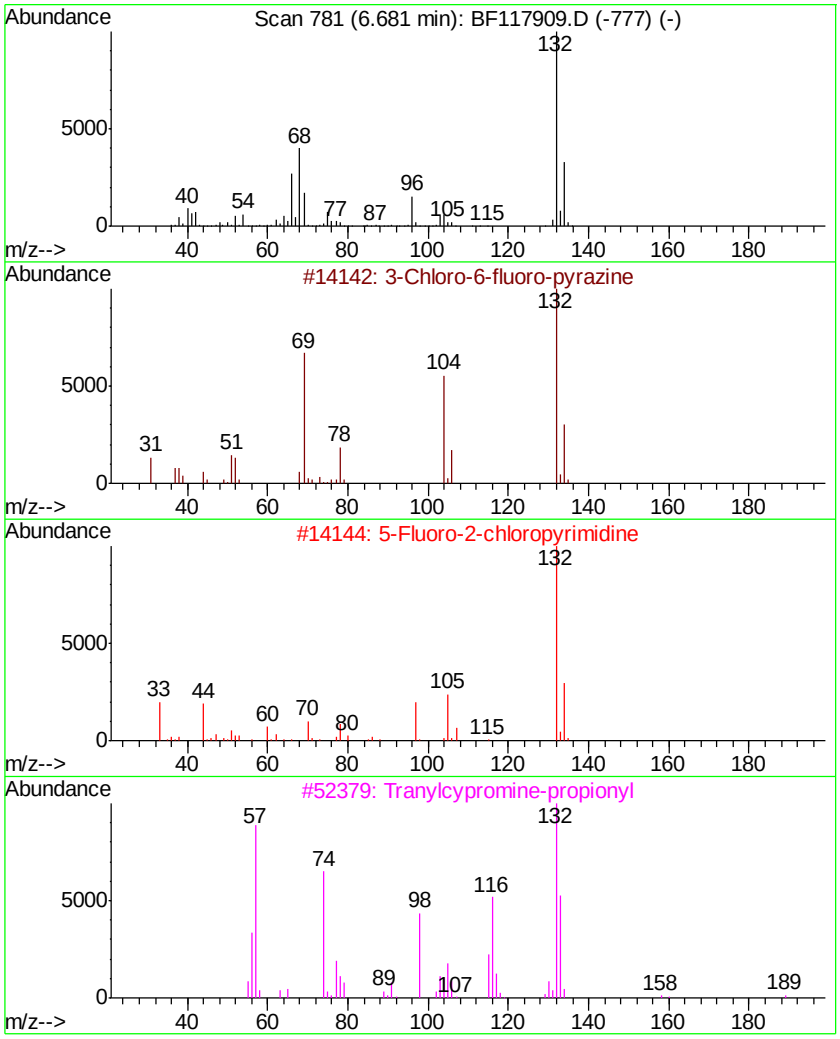
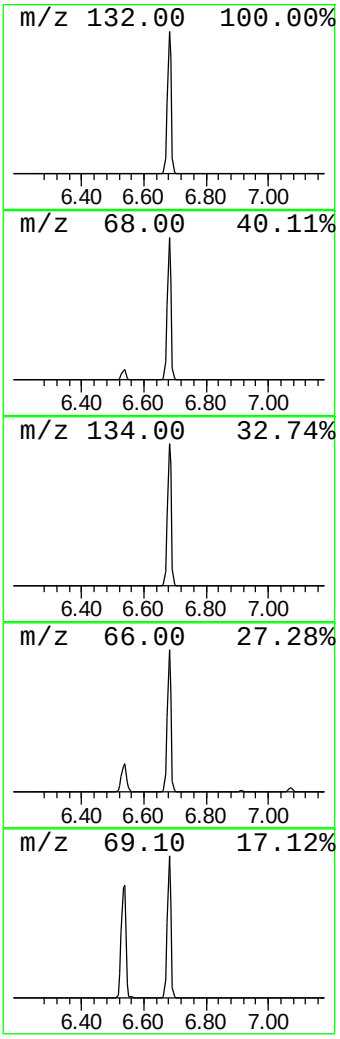
****

Peak Number 3 unknown6.68 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.68	75.70 ng	3002110	1,4-Dichlorobenzene-d4	6.92

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	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	Benzene, 1-ethenyl-3,5-dimethyl-	132	C10H12	005379-20-4	9





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Instrument : BNA_F
ClientSampleId : RBR200027-1A-415

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF111319.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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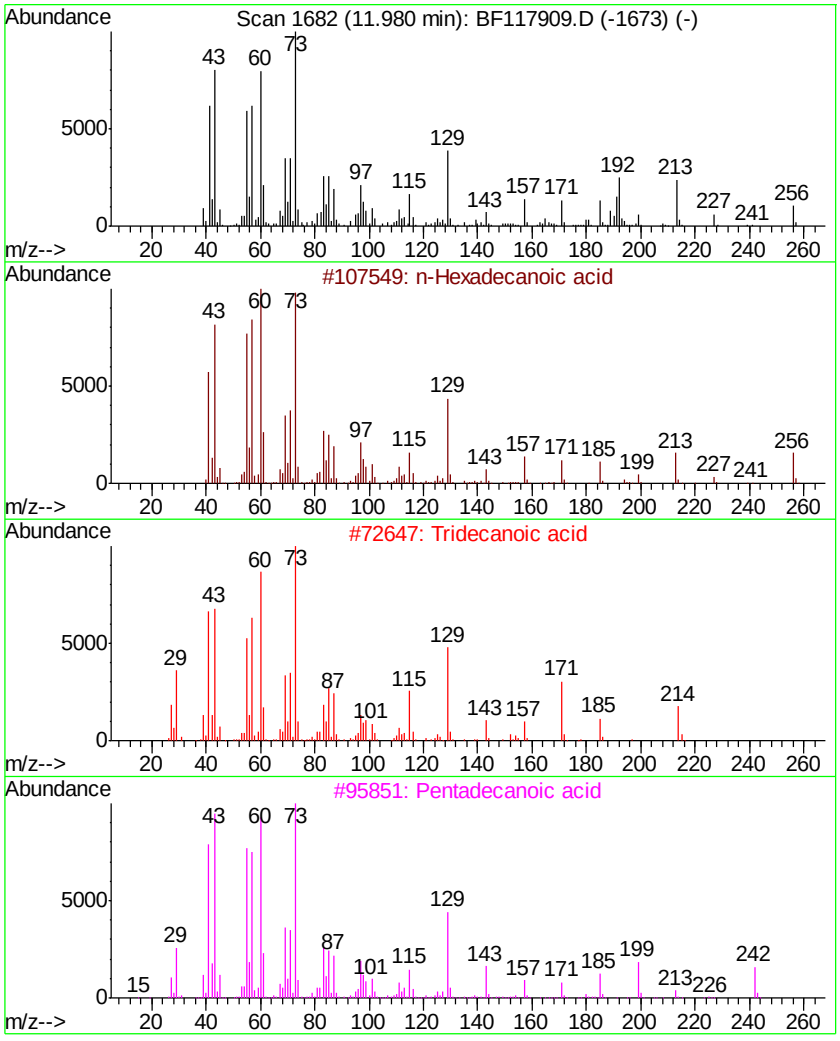
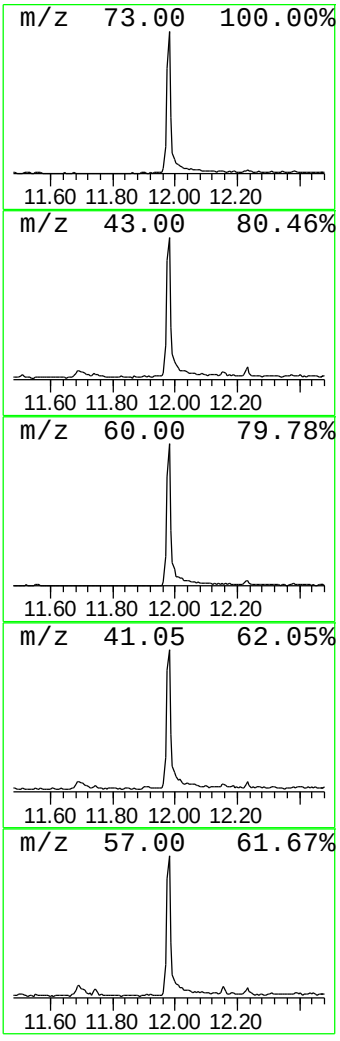
Peak Number 5 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.98	10.05 ng	836783	Phenanthrene-d10	11.46

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	95
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	81
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	76
5	n-Decanoic acid	172	C10H20O2	000334-48-5	64





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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF111319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

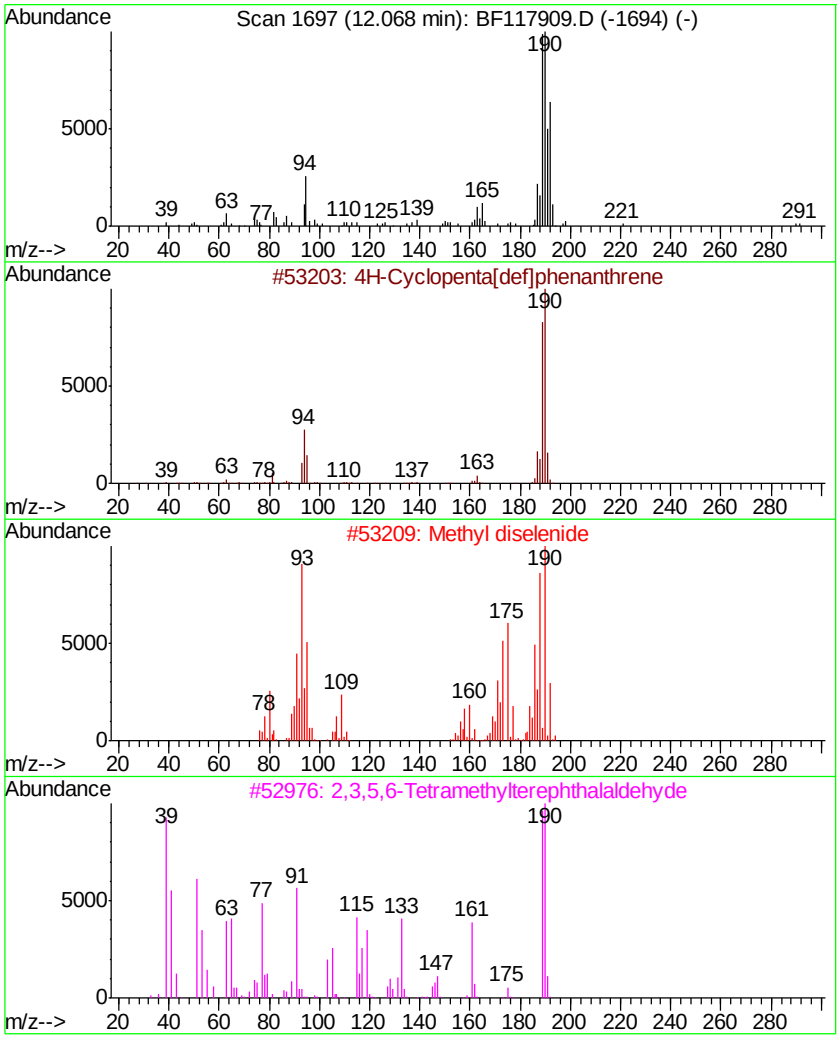
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

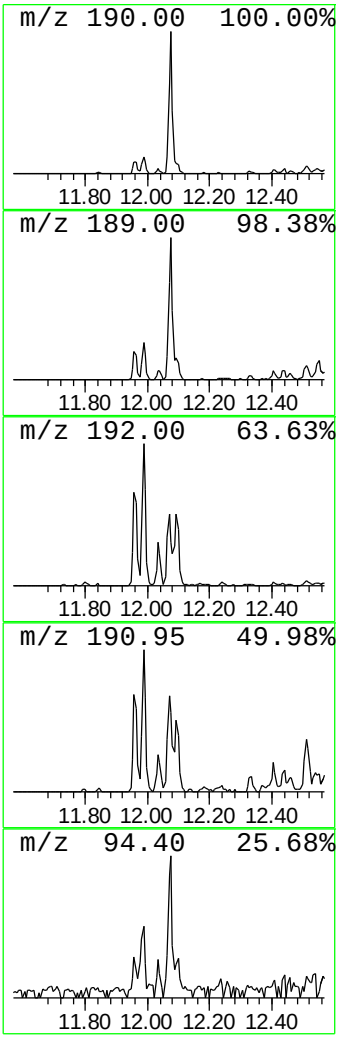
****

Peak Number 6 4H-Cyclopenta[def]phenanthrene Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.07	2.45 ng	203743	Phenanthrene-d10	11.46

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	83
2	Methyl diselenide	190	C2H6Se2	007101-31-7	55
3	2,3,5,6-Tetramethylterephthalald...	190	C12H14O2	007072-01-7	53
4	2,2'-Bis(4,5-dimethylimidazole)	190	C10H14N4	069286-06-2	45
5	1,4-Naphthalenedione, 2,5-dihydr...	190	C10H6O4	004923-55-1	32





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Data File : BF117909.D
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Sample : K5932-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RBR200027-1A-415

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF111319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

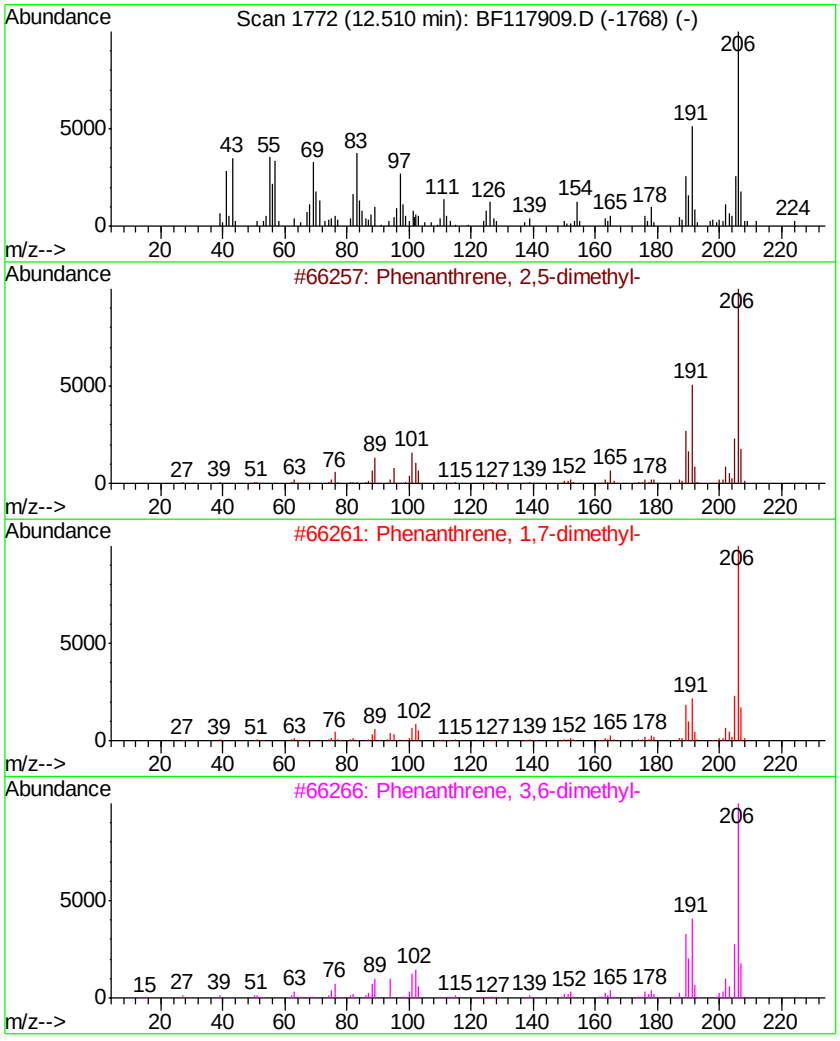
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

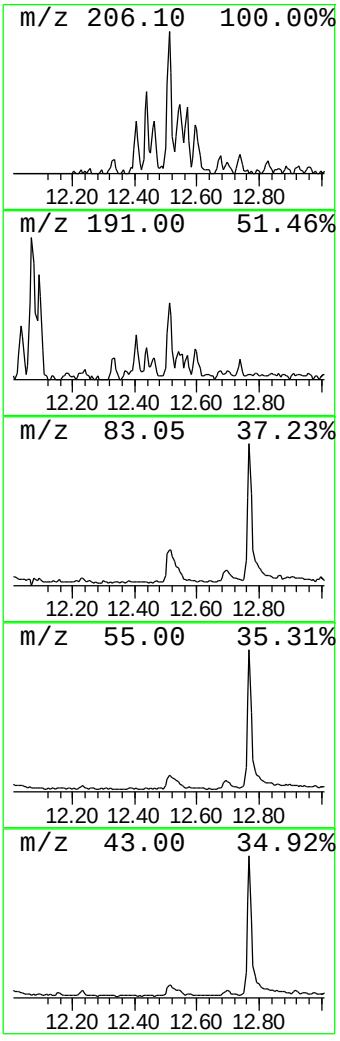
****

Peak Number 7 Phenanthrene, 2,5-dimethyl- Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.51	2.04 ng	169798	Phenanthrene-d10	11.46

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenanthrene, 2,5-dimethyl-	206	C16H14	003674-66-6	95
2	Phenanthrene, 1,7-dimethyl-	206	C16H14	000483-87-4	95
3	Phenanthrene, 3,6-dimethyl-	206	C16H14	001576-67-6	94
4	di-p-Tolylacetylene	206	C16H14	002789-88-0	92
5	9,10-Dimethylanthracene	206	C16H14	000781-43-1	90





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF112119\
Data File : BF117909.D
Acq On : 21 Nov 2019 13:53
Operator : JU
Sample : K5932-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RBR200027-1A-415

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF111319.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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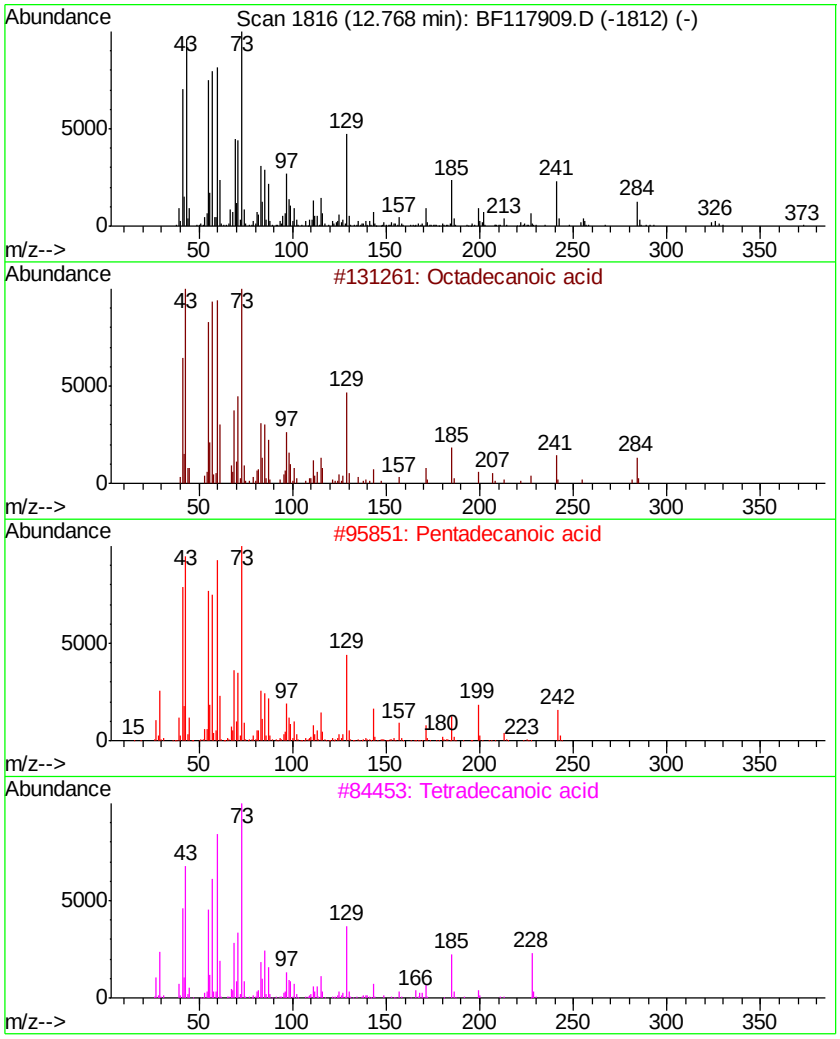
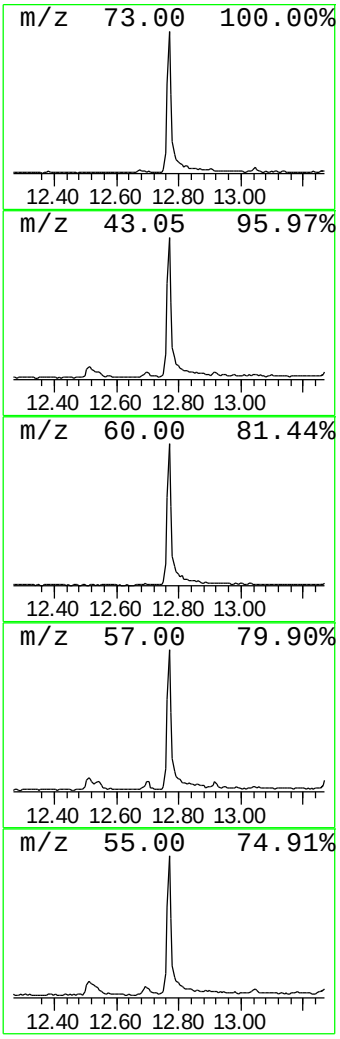
Peak Number 8 Octadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.77	12.34 ng	1027230	Phenanthrene-d10	11.46

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	93
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	83
4	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	80
5	Tridecanoic acid	214	C13H26O2	000638-53-9	74





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Acq On : 21 Nov 2019 13:53
Operator : JU
Sample : K5932-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RBR200027-1A-415

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF111319.M
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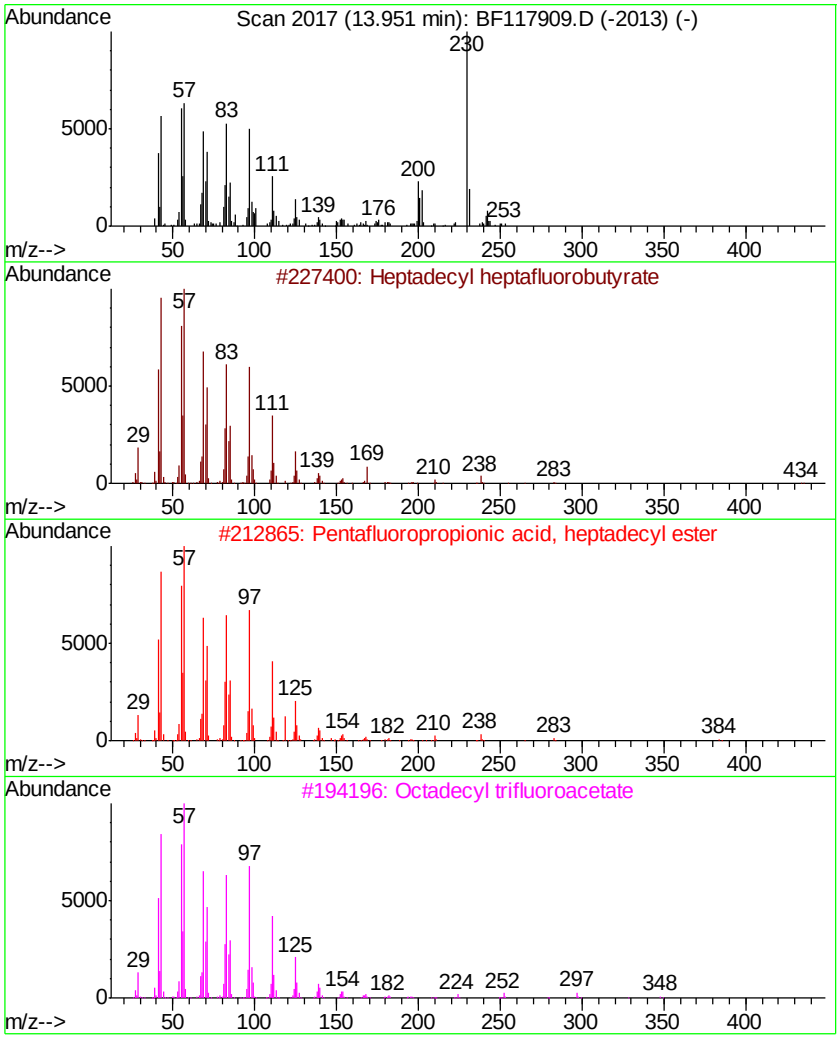
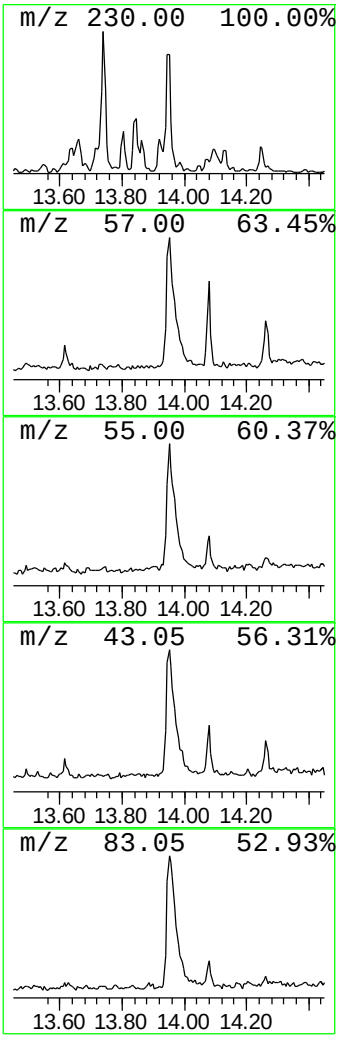
Peak Number 9 Heptadecyl heptafluorobutyrate Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.95	4.12 ng	519647	Chrysene-d12	14.10

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	89
2	Pentafluoropropionic acid, hepta...	402	C20H35F5O2	959218-78-1	89
3	Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	89
4	1-Heneicosanol	312	C21H44O	015594-90-8	84
5	Heptafluorobutyric acid, n-octad...	466	C22H37F7O2	000400-57-7	83





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Operator : JU
Sample : K5932-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RBR200027-1A-415

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF111319.M
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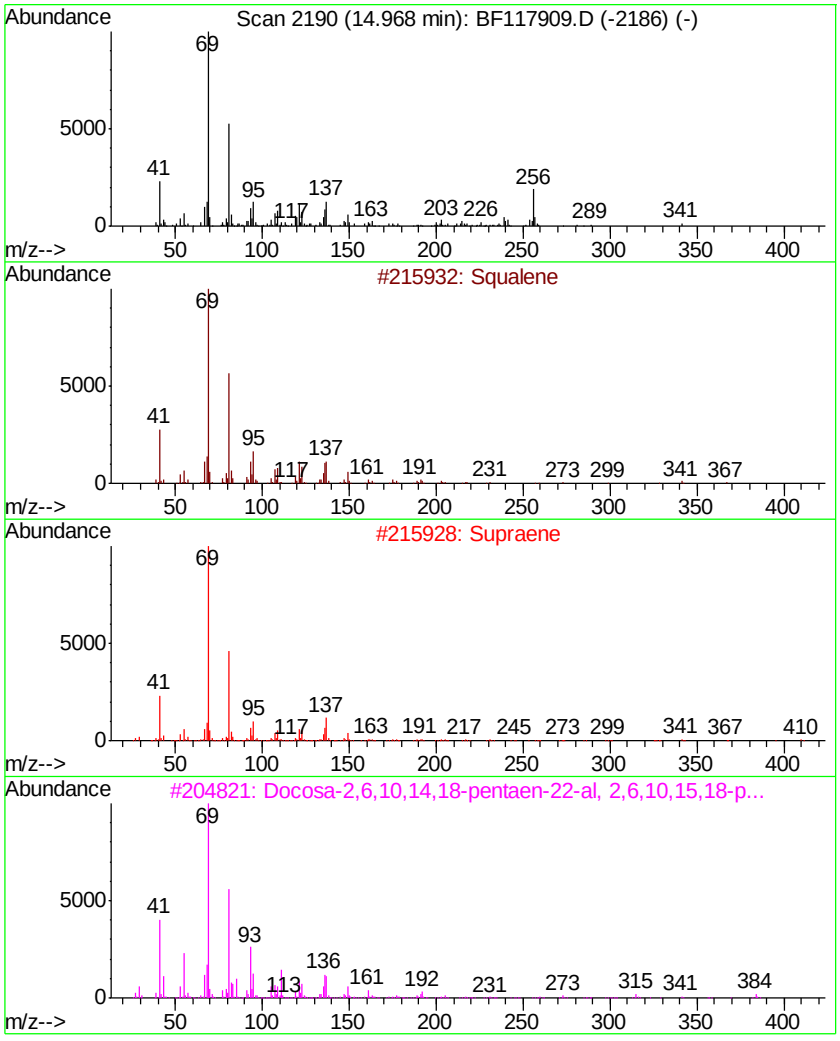
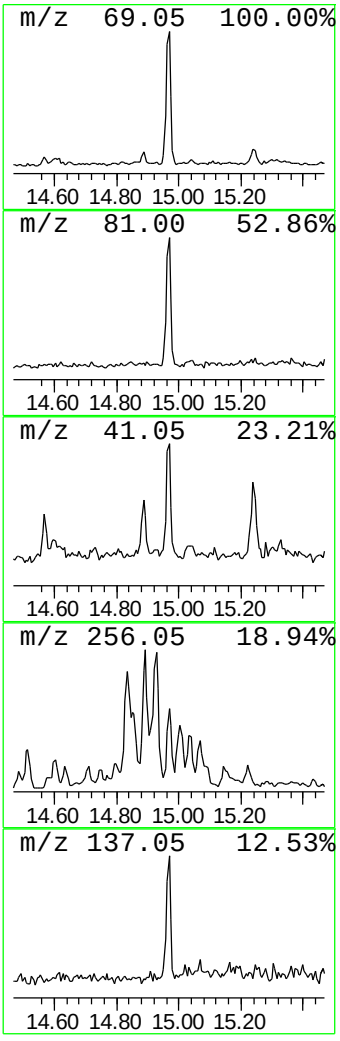
Peak Number 10 Squalene Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.97	2.45 ng	175679	Perylene-d12	15.62

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Squalene	410	C30H50	000111-02-4	81
2	Supraene	410	C30H50	007683-64-9	74
3	Docosa-2,6,10,14,18-pentaen-22-a...	384	C27H44O	1000163-04-7	72
4	Hexadeca-2,6,10,14-tetraen-1-ol,...	290	C20H34O	007614-21-3	64
5	Propanoic acid, 2,2-dimethyl-, [...	306	C20H34O2	1000164-38-8	59





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Sample : K5932-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RBR200027-1A-415

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF111319.M
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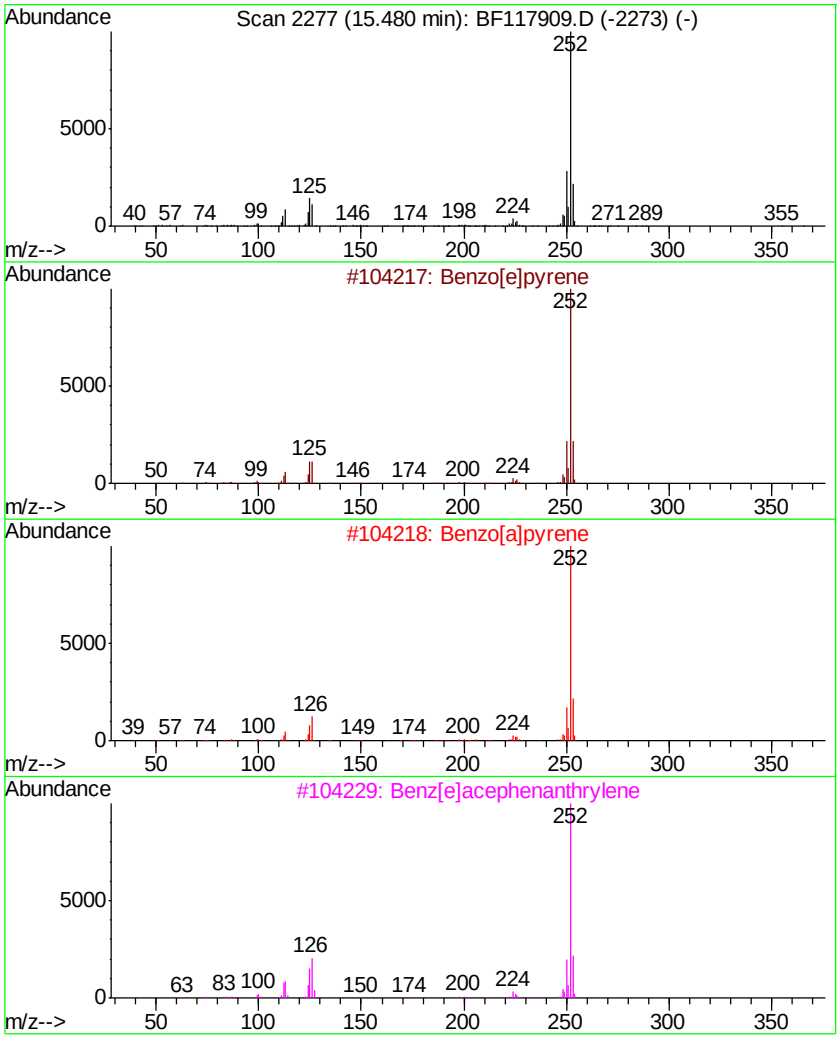
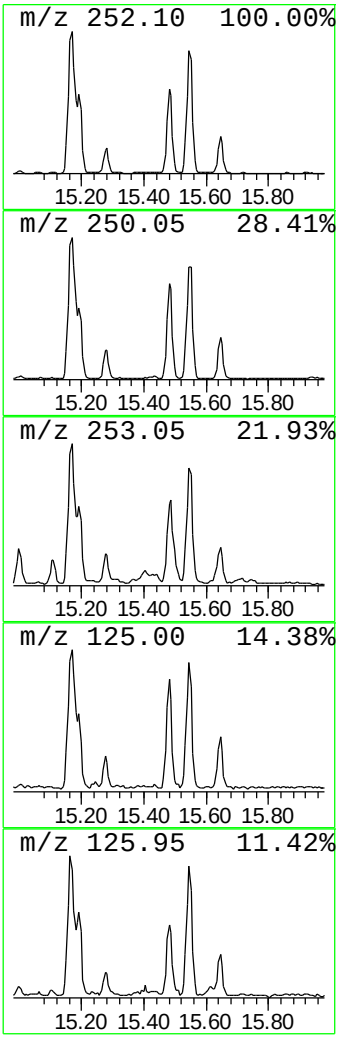
Peak Number 11 Benzo[e]pyrene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.48	7.50 ng	538965	Perylene-d12	15.62

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





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Sample : K5932-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RBR200027-1A-415

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF111319.M
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TIC Integration Parameters: LSCINT.P

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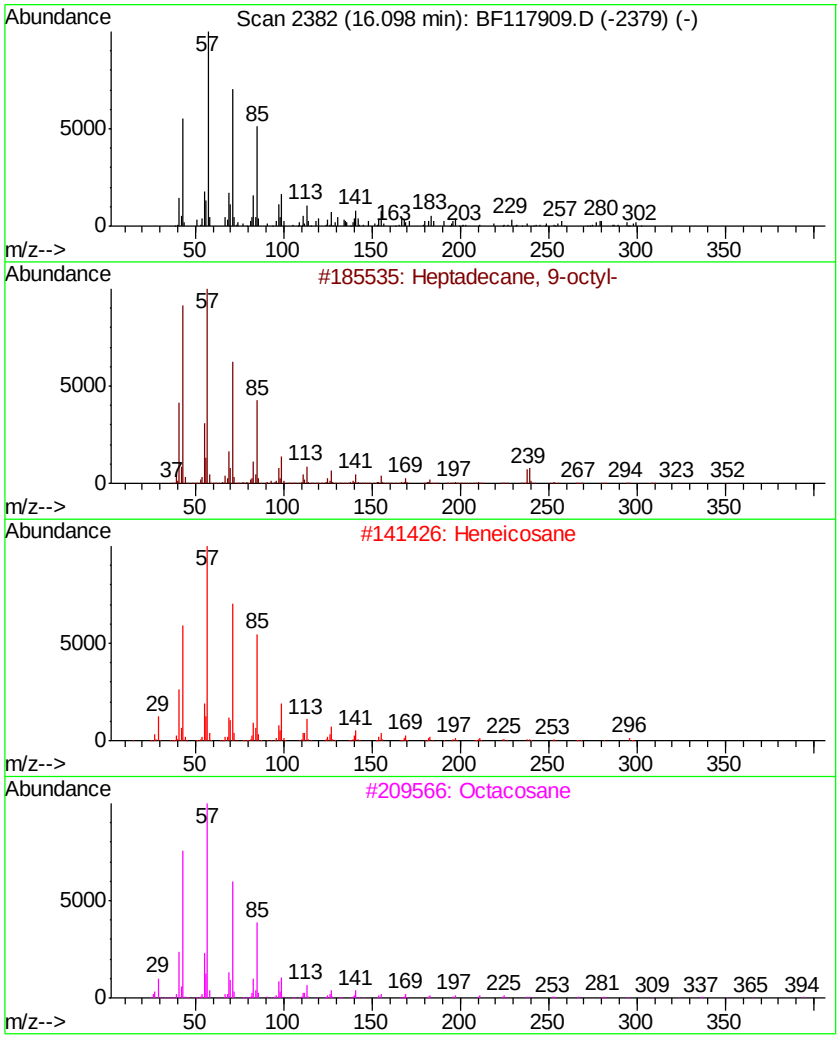
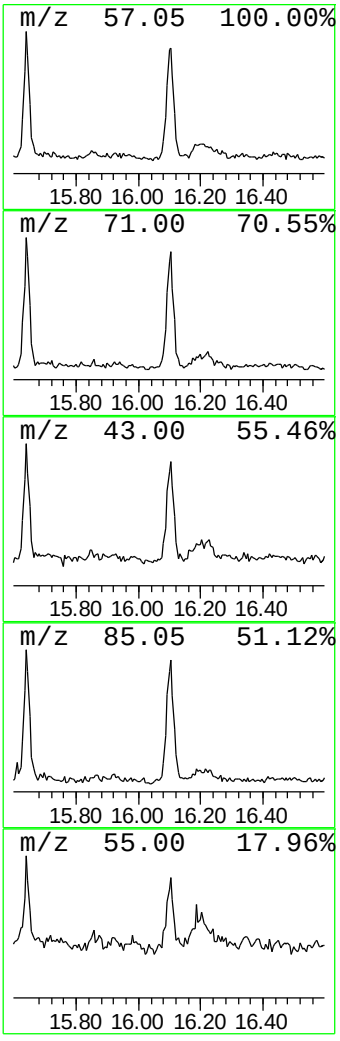
Peak Number 12 Heptadecane, 9-octyl- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.10	2.20 ng	157950	Perylene-d12	15.62

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	83
2	Heneicosane	296	C21H44	000629-94-7	83
3	Octacosane	394	C28H58	000630-02-4	83
4	Docosane	310	C22H46	000629-97-0	80
5	Tetratetracontane	619	C44H90	007098-22-8	68





Tentatively Identified Compound (LSC) summary

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ALS Vial : 11 Sample Multiplier: 1

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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
Butane, 2-methoxy...	2.17	24.1	ng	956049	1	6.92	793142	20.0
2-Pentanone, 4-hy...	5.12	12.6	ng	499145	1	6.92	793142	20.0
unknown6.68	6.68	75.7	ng	3002110	1	6.92	793142	20.0
n-Hexadecanoic acid	11.98	10.1	ng	836783	4	11.46	1664790	20.0
4H-Cyclopenta[def...	12.07	2.5	ng	203743	4	11.46	1664790	20.0
Phenanthrene, 2,5...	12.51	2.0	ng	169798	4	11.46	1664790	20.0
Octadecanoic acid	12.77	12.3	ng	1027230	4	11.46	1664790	20.0
Heptadecyl heptaf...	13.95	4.1	ng	519647	5	14.10	2519830	20.0
Squalene	14.97	2.5	ng	175679	6	15.62	1436990	20.0
Benzo[e]pyrene	15.48	7.5	ng	538965	6	15.62	1436990	20.0
Heptadecane, 9-oc...	16.10	2.2	ng	157950	6	15.62	1436990	20.0