LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF110819\
Data File : BF117749.D
Acq On : 8 Nov 2019 23:25
Operator : JU
Sample : K5668-01 2X
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : HD-01-110619

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-BF110619.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	2.204	15	20	37	rVB	756097	1081516	23.76%	1.711%
2	5.140	514	519	525	rVB	702782	781643	17.17%	1.237%
3	5.534	582	586	590	rBV	3743986	3598448	79.05%	5.694%
4	6.539	752	757	762	rBV	3827551	3966759	87.14%	6.277%
5	6.692	779	783	786	rBV	4650371	3954565	86.87%	6.257%
6	6.928	819	823	826	rBV	2759110	2172455	47.73%	3.438%
7	7.086	846	850	853	rBV	3748215	3107844	68.27%	4.918%
8	7.486	914	918	921	rBV	2915658	2397517	52.67%	3.794%
9	8.216	1038	1042	1045	rBV	3538057	2887477	63.43%	4.569%
10	9.292	1221	1225	1228	rBV	5707881	4552018	100.00%	7.203%
11	9.680	1289	1291	1296	rBV	476396	434718	9.55%	0.688%
12	9.833	1315	1317	1321	rBV	95420	95571	2.10%	0.151%
13	9.869	1321	1323	1327	rVV	54485	67883	1.49%	0.107%
14	9.974	1335	1341	1345	rBV	3781020	3413373	74.99%	5.401%
15	10.174	1371	1375	1380	rVB2	49961	68546	1.51%	0.108%
16	10.404	1412	1414	1417	rVB	79937	62511	1.37%	0.099%
17	10.522	1431	1434	1440	rVB2	80268	87827	1.93%	0.139%
18	10.763	1471	1475	1480	rBV	3398358	2956768	64.96%	4.679%
19	10.880	1492	1495	1500	rVB2	144527	178627	3.92%	0.283%
20	11.074	1524	1528	1530	rBV2	52797	57474	1.26%	0.091%
21	11.333	1566	1572	1575	rBV3	97820	147295	3.24%	0.233%
22	11.363	1575	1577	1582	rVB	101549	93892	2.06%	0.149%
23	11.469	1591	1595	1597	rBV	3937589	3377006	74.19%	5.344%
24	11.492	1597	1599	1602	rVV	845837	636369	13.98%	1.007%
25	11.539	1604	1607	1610	rVB	246374	219595	4.82%	0.347%
26	11.692	1629	1633	1635	rBV	113672	116692	2.56%	0.185%
27	11.763	1642	1645	1647	rVB2	98531	83630	1.84%	0.132%
28	11.857	1658	1661	1664	rBV	261342	197624	4.34%	0.313%
29	11.921	1668	1672	1674	rBV5	46419	57314	1.26%	0.091%
30	11.968	1677	1680	1681	rVV	217824	177737	3.90%	0.281%
31	11.992	1681	1684	1690	rVV2	837910	920828	20.23%	1.457%
32	12.045	1690	1693	1695	rVV	105297	95939	2.11%	0.152%
33	12.080	1696	1699	1702	rVV2	273808	322702	7.09%	0.511%
34	12.104	1702	1703	1708	rVB	162906	99751	2.19%	0.158%

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Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : HD-01-110619

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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Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	12.168	1711	1714	1717	rVB	113571	98542	2.16%	0.156%
36	12.245	1724	1727	1729	rBV3	106053	104598	2.30%	0.166%
37	12.263	1729	1730	1732	rVB	87728	63788	1.40%	0.101%
38	12.398	1750	1753	1754	rBV3	58995	58088	1.28%	0.092%
39	12.445	1759	1761	1763	rBV	79826	70481	1.55%	0.112%
40	12.521	1771	1774	1776	rBV	190306	187598	4.12%	0.297%
41	12.551	1776	1779	1780	rVV2	538884	548346	12.05%	0.868%
42	12.568	1780	1782	1786	rVV	971916	838963	18.43%	1.328%
43	12.604	1786	1788	1793	rVB2	115152	110084	2.42%	0.174%
44	12.651	1794	1796	1798	rBV2	92666	71563	1.57%	0.113%
45	12.680	1798	1801	1807	rBV	1398349	1361296	29.91%	2.154%
46	12.774	1814	1817	1822	rBV2	275964	300201	6.59%	0.475%
47	12.915	1834	1841	1846	rBV2	1197041	1448435	31.82%	2.292%
48	13.057	1861	1865	1868	rVB	4538216	3782281	83.09%	5.985%
49	13.133	1874	1878	1885	rBV3	146225	252141	5.54%	0.399%
50	13.221	1890	1893	1894	rVV3	110965	118418	2.60%	0.187%
51	13.239	1894	1896	1899	rVB	235164	202479	4.45%	0.320%
52	13.286	1902	1904	1906	rBV	129291	127585	2.80%	0.202%
53	13.310	1906	1908	1910	rVB	149690	112191	2.46%	0.178%
54	13.345	1911	1914	1917	rVV2	214594	199352	4.38%	0.315%
55	13.439	1928	1930	1932	rVB	133275	92048	2.02%	0.146%
56	13.468	1932	1935	1939	rBV	127261	144199	3.17%	0.228%
57	13.633	1961	1963	1967	rVB2	135256	114428	2.51%	0.181%
58	13.745	1980	1982	1987	rVB	164022	160694	3.53%	0.254%
59	13.892	2005	2007	2009	rBV	99274	66342	1.46%	0.105%
60	13.957	2014	2018	2029	rVB4	532091	723323	15.89%	1.145%
61	14.115	2040	2045	2047	rBV2	2540282	2991636	65.72%	4.734%
62	14.139	2047	2049	2051	rVB	586002	419937	9.23%	0.664%
63	14.280	2070	2073	2079	rVB3	230745	274181	6.02%	0.434%
64	14.586	2122	2125	2129	rBV2	355545	357704	7.86%	0.566%
65	14.904	2177	2179	2182	rVB	265849	229538	5.04%	0.363%
66	15.174	2222	2225	2228	rBV	484508	722412	15.87%	1.143%
67	15.262	2236	2240	2242	rBV	298497	378829	8.32%	0.599%
68	15.492	2276	2279	2285	rVB	383279	500222	10.99%	0.792%
69	15.556	2287	2290	2294	rVV	459775	563203	12.37%	0.891%
70	15.627	2297	2302	2305	rVV	1795776	2327760	51.14%	3.683%
71	15.656	2305	2307	2315	rVB3	417022	605188	13.29%	0.958%

LSC Area Percent Report

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Integrator: RTE
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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

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Sum of corrected areas: 63197988

LSC Report - Integrated Chromatogram

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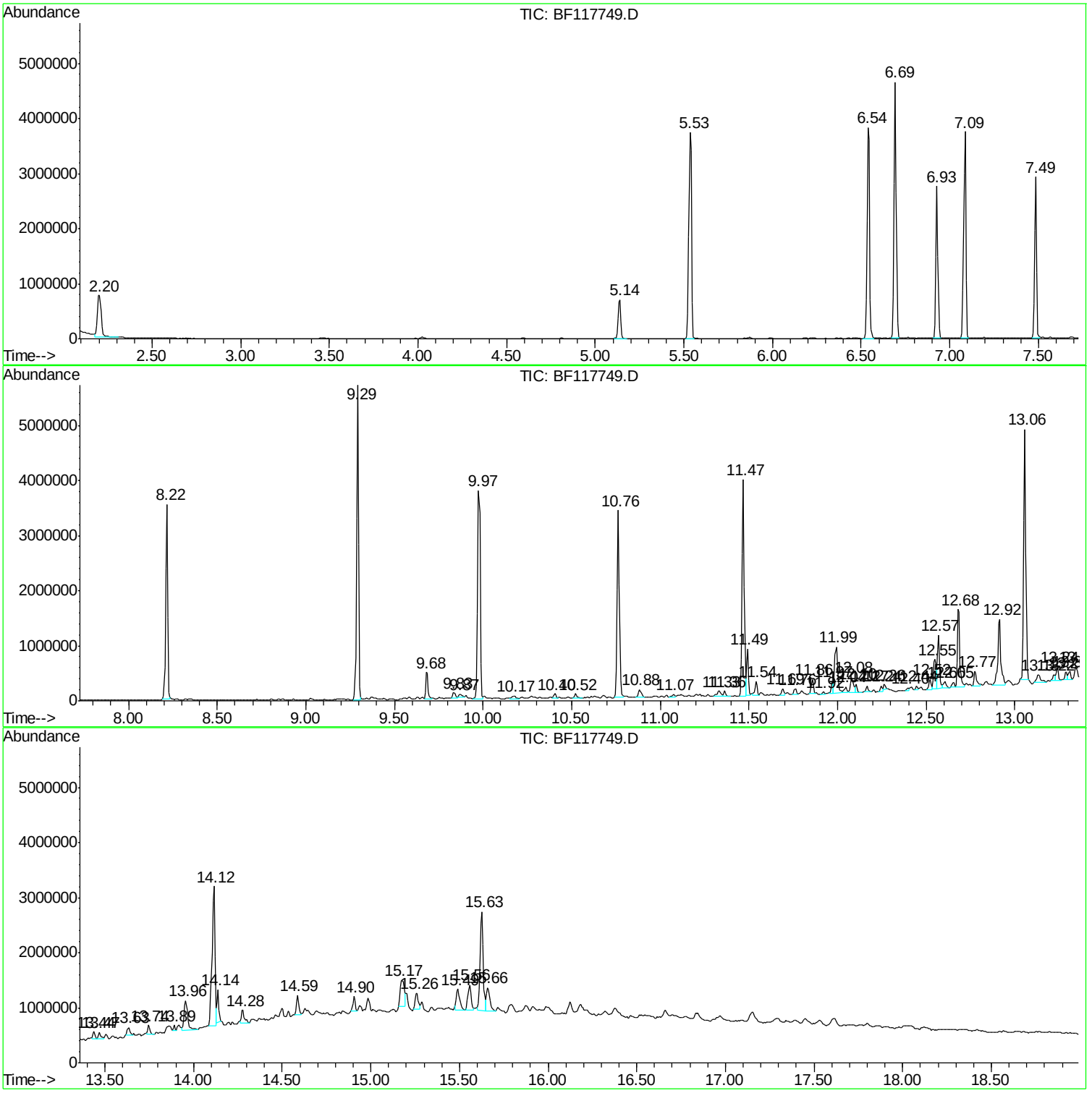
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : HD-01-110619

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110619.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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Data File : BF117749.D
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Operator : JU
Sample : K5668-01 2X
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : HD-01-110619

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110619.M
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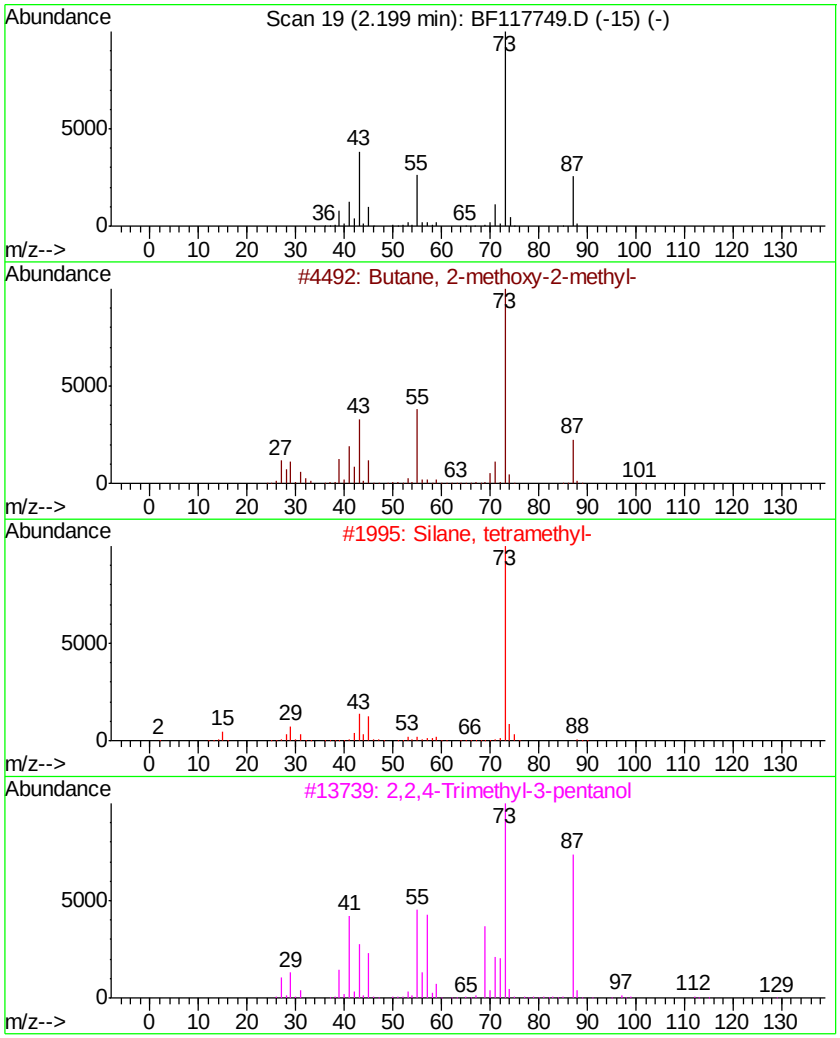
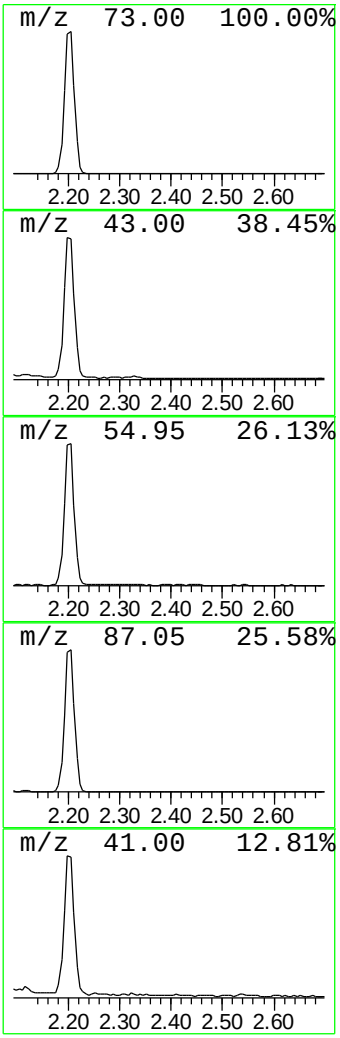
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.20	9.96 ng	1081520	1,4-Dichlorobenzene-d4	6.93

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2	Silane, tetramethyl-	88	C4H12Si	000075-76-3	43
3	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
4	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
5	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17





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Sample : K5668-01 2X
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ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : HD-01-110619

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110619.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

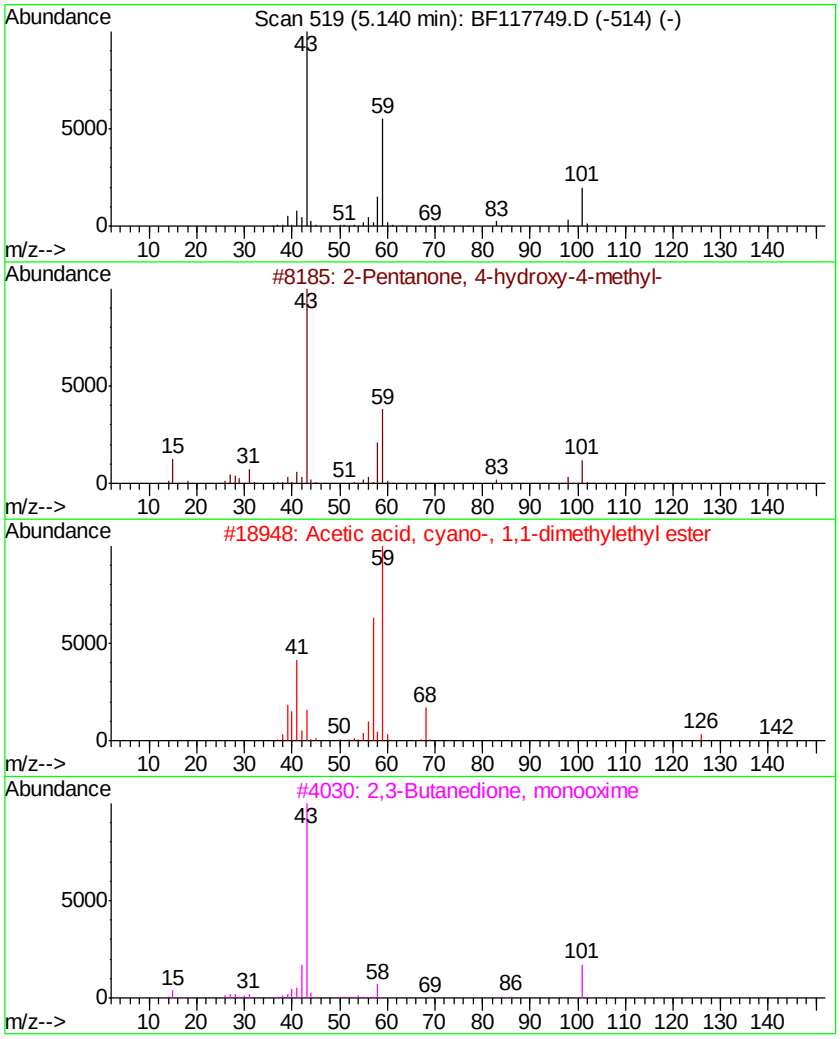
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

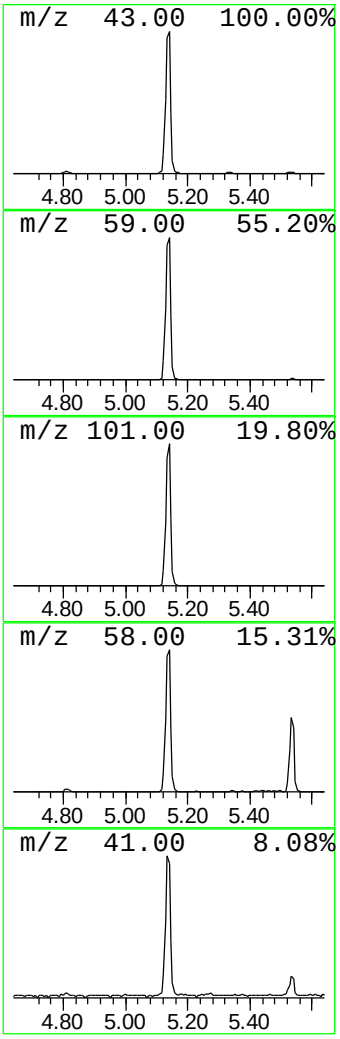
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.14	7.20 ng	781643	1,4-Dichlorobenzene-d4	6.93

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5	1,2-Butanediol	90	C4H10O2	000584-03-2	9





Library Search Compound Report

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Acq On : 8 Nov 2019 23:25
Operator : JU
Sample : K5668-01 2X
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : HD-01-110619

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110619.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

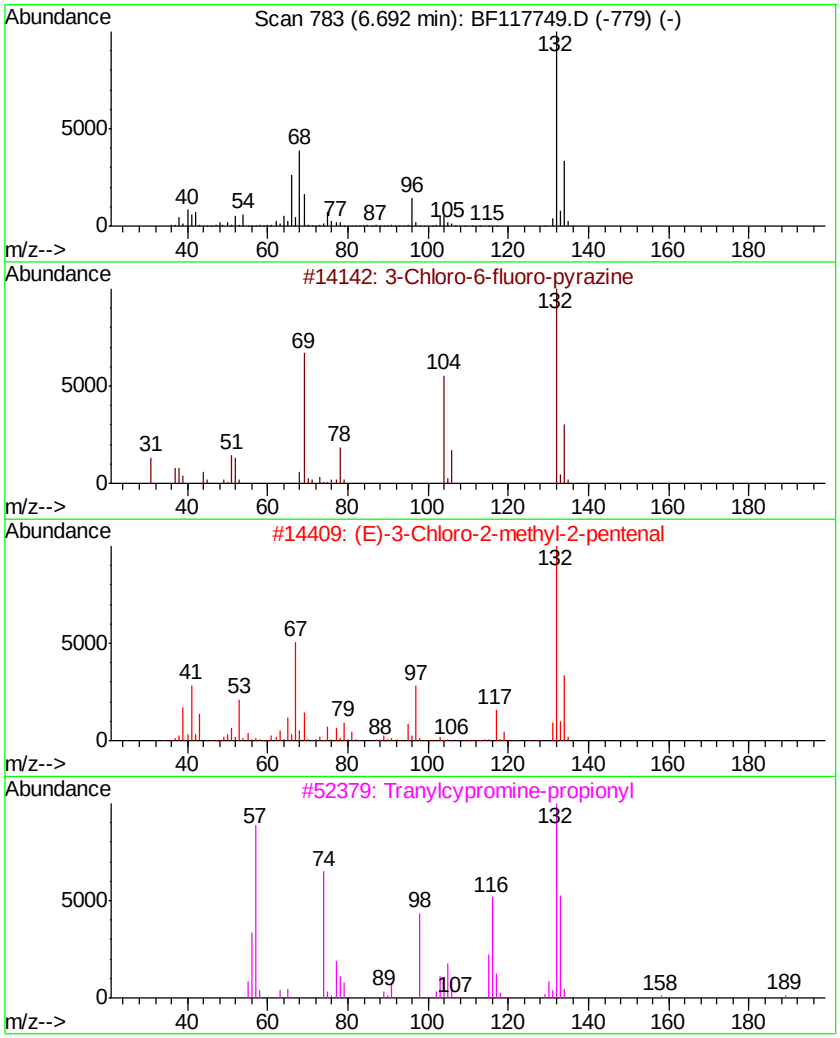
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

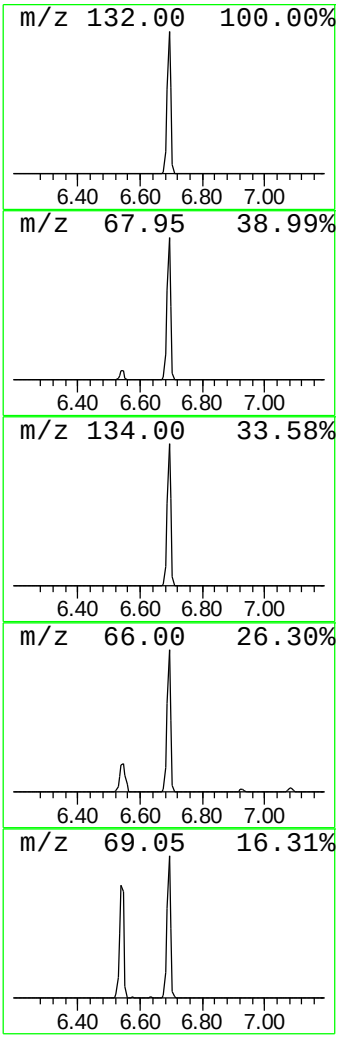
****

Peak Number 3 unknown6.69 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.69	36.41 ng	3954570	1,4-Dichlorobenzene-d4	6.93

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	Benzene, 1-ethenyl-3,5-dimethyl-	132	C10H12	005379-20-4	9





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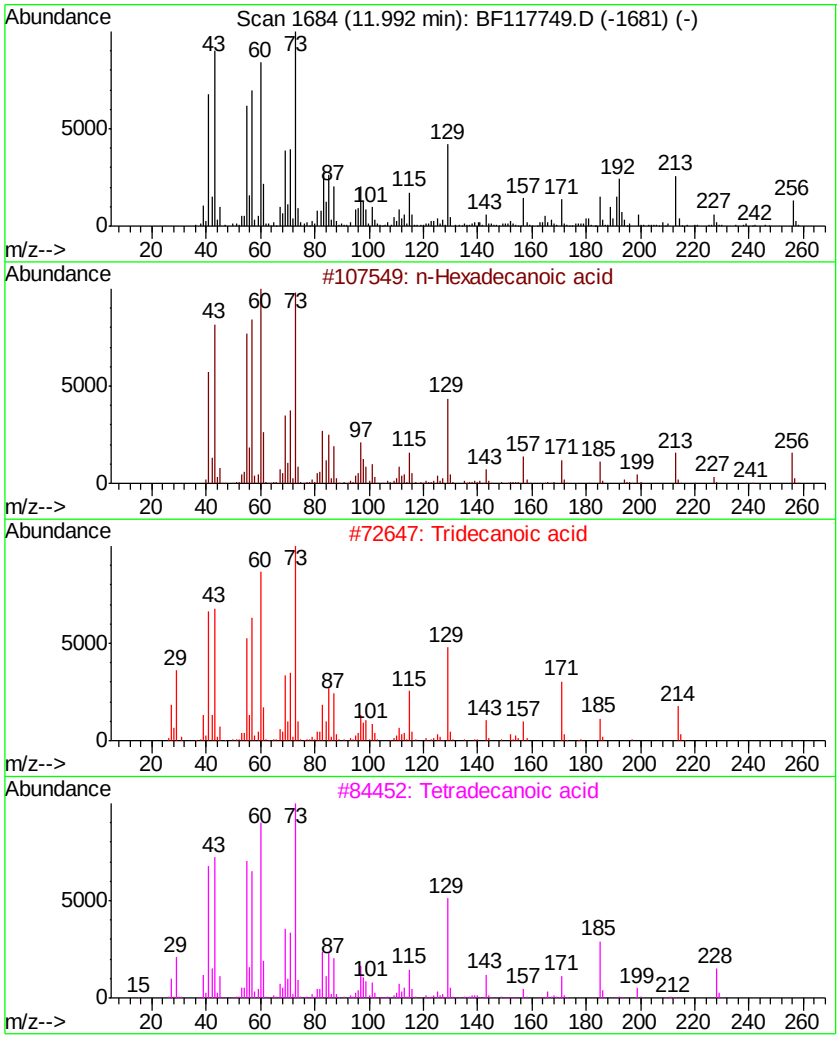
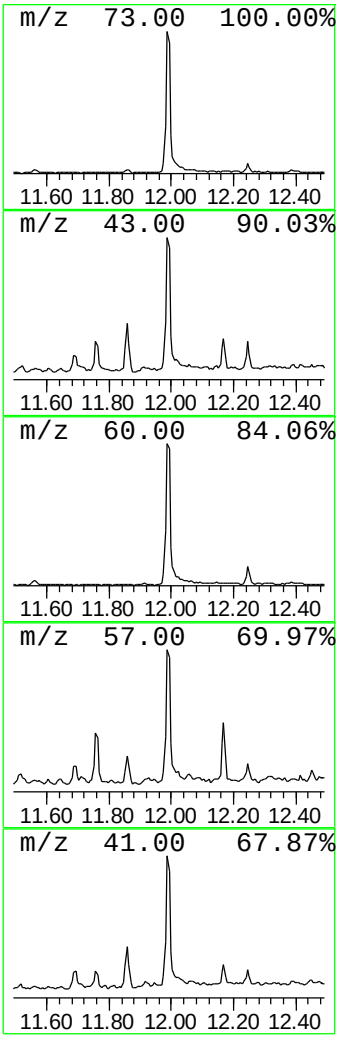
****

Peak Number 5 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.99	5.45 ng	920828	Phenanthrene-d10	11.47

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	93
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	93
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
5	n-Decanoic acid	172	C10H20O2	000334-48-5	70





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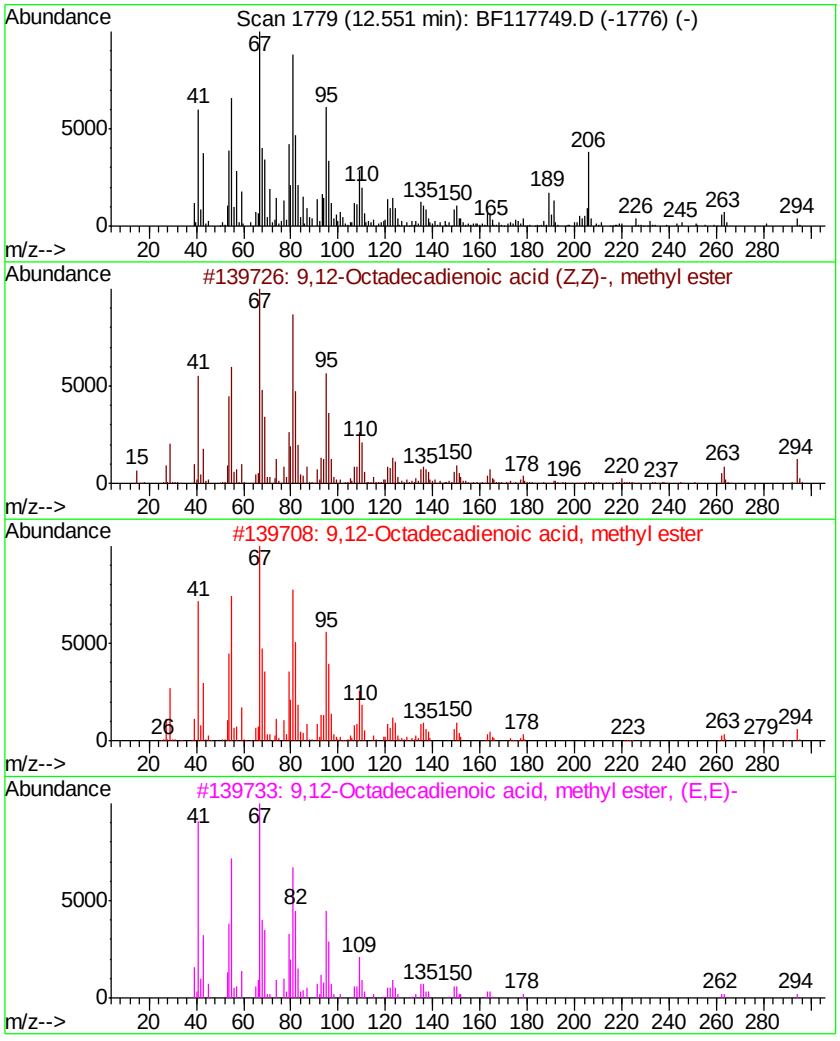
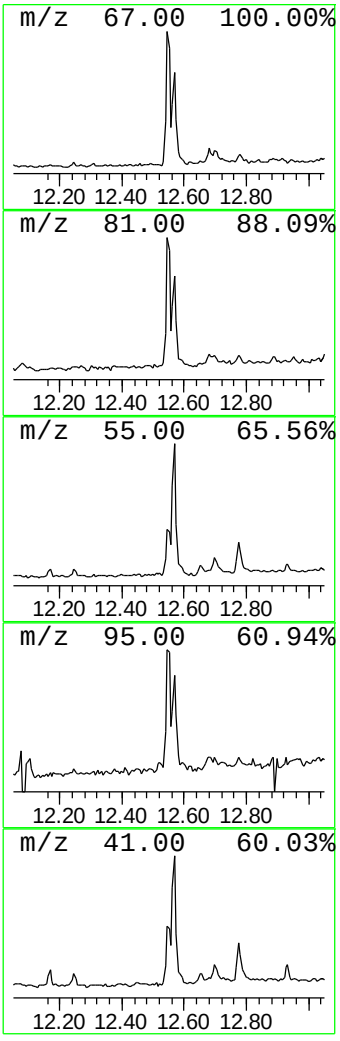
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 9,12-Octadecadienoic acid (... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.55	3.25 ng	548346	Phenanthrene-d10	11.47

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9,12-Octadecadienoic acid (Z,Z)-...	294	C19H34O2	000112-63-0	99
2	9,12-Octadecadienoic acid, methy...	294	C19H34O2	002462-85-3	99
3	9,12-Octadecadienoic acid, methy...	294	C19H34O2	002566-97-4	99
4	10,13-Octadecadienoic acid, meth...	294	C19H34O2	056554-62-2	98
5	Methyl 10-trans,12-cis-octadecad...	294	C19H34O2	1000336-44-2	98





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Instrument : BNA_F
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110619.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

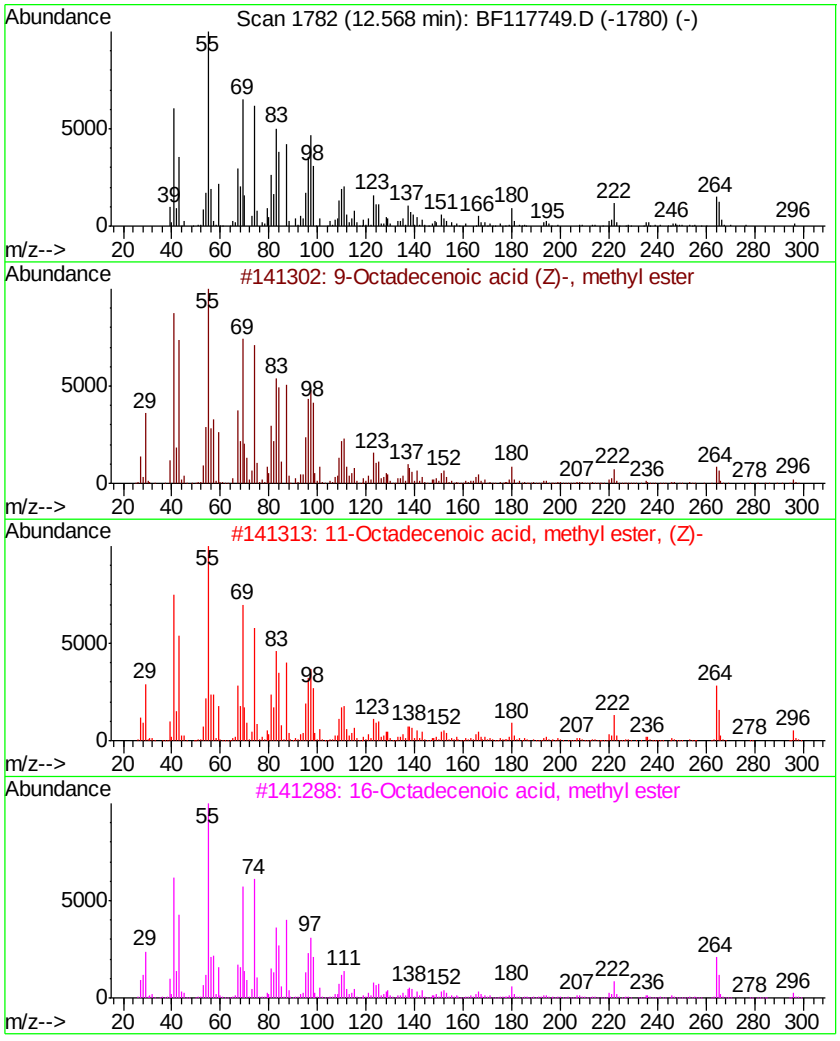
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

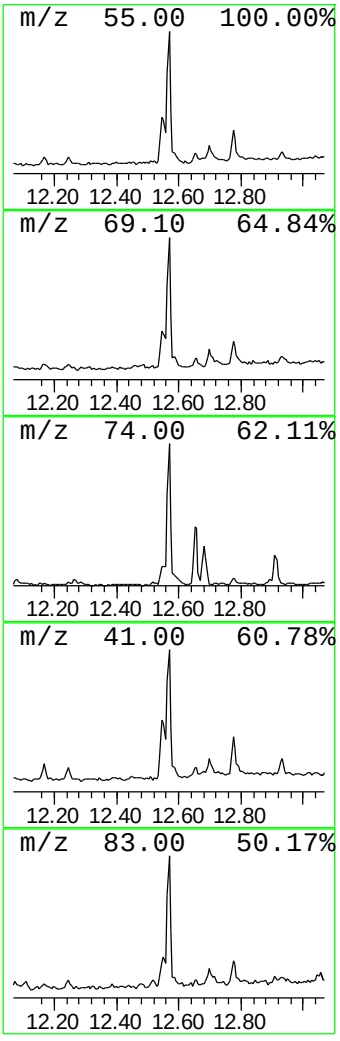
****

Peak Number 7 9-Octadecenoic acid (Z)-, m... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.57	4.97 ng	838963	Phenanthrene-d10	11.47

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenoic acid (Z)-, methyl...	296	C19H36O2	000112-62-9	99
2	11-Octadecenoic acid, methyl est...	296	C19H36O2	001937-63-9	99
3	16-Octadecenoic acid, methyl ester	296	C19H36O2	056554-49-5	99
4	10-Octadecenoic acid, methyl ester	296	C19H36O2	013481-95-3	99
5	9-Octadecenoic acid, methyl ester	296	C19H36O2	002462-84-2	99





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Instrument : BNA_F
ClientSampleId : HD-01-110619

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110619.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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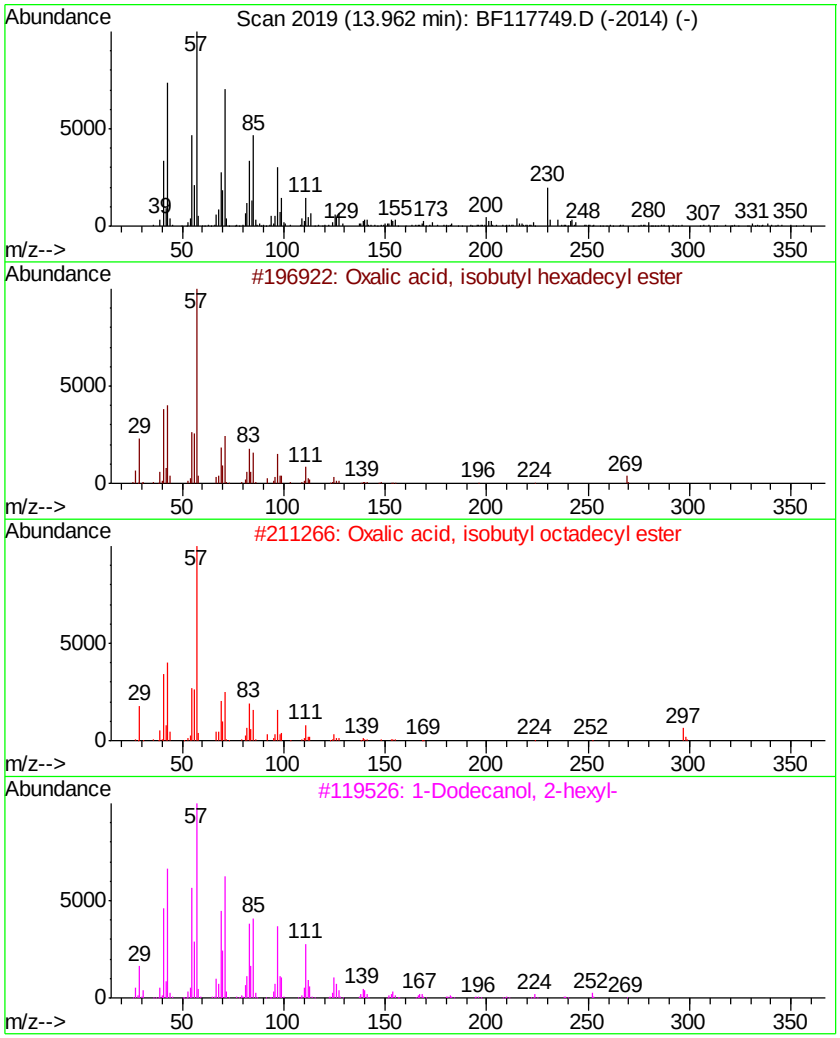
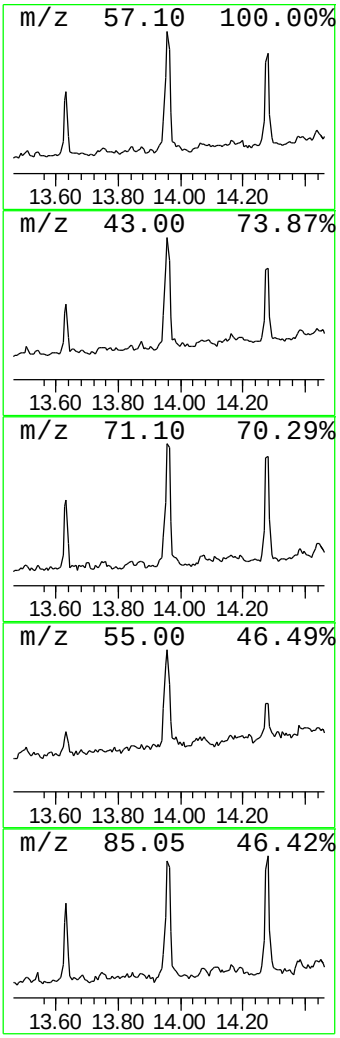
Peak Number 8 Oxalic acid, isobutyl hexad... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.96	4.84 ng	723323	Chrysene-d12	14.12

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oxalic acid, isobutyl hexadecyl ...	370	C22H42O4	1000309-38-1	70
2	Oxalic acid, isobutyl octadecyl ...	398	C24H46O4	1000309-38-3	62
3	1-Dodecanol, 2-hexyl-	270	C18H38O	110225-00-8	55
4	1-Decanol, 2-hexyl-	242	C16H34O	002425-77-6	55
5	11H-Benzo[a]fluoren-11-one	230	C17H10O	000479-79-8	53





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF110819\
Data File : BF117749.D
Acq On : 8 Nov 2019 23:25
Operator : JU
Sample : K5668-01 2X
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : HD-01-110619

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110619.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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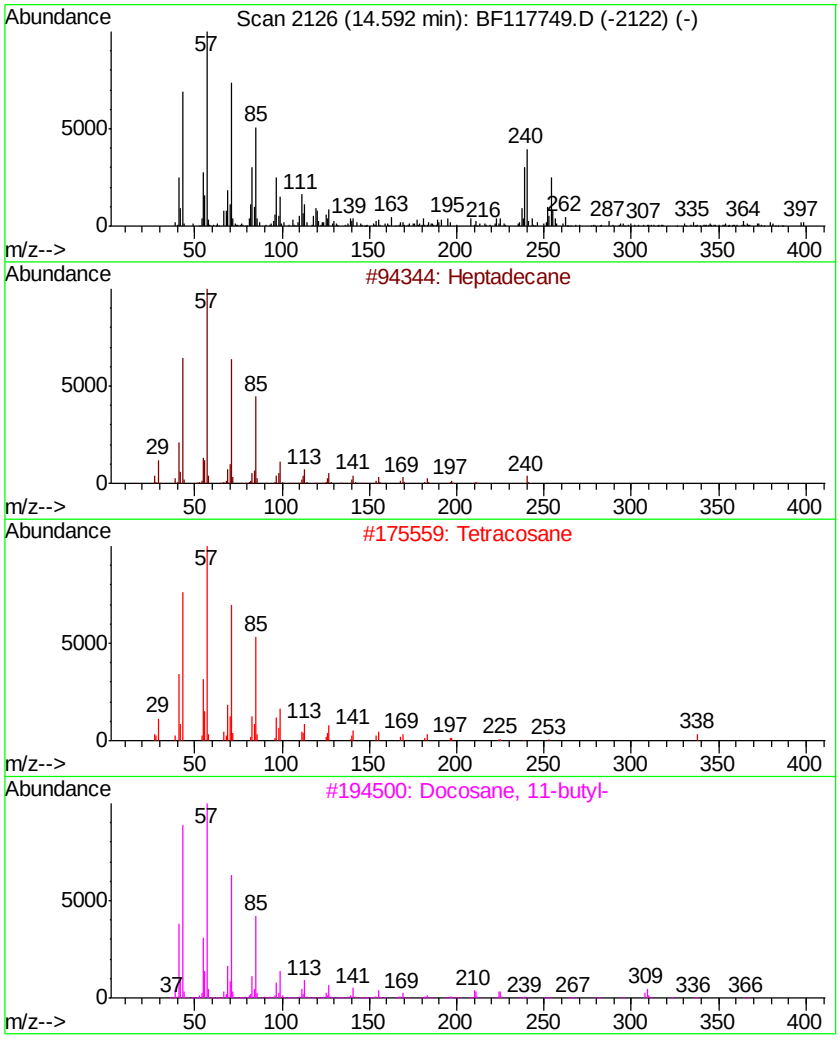
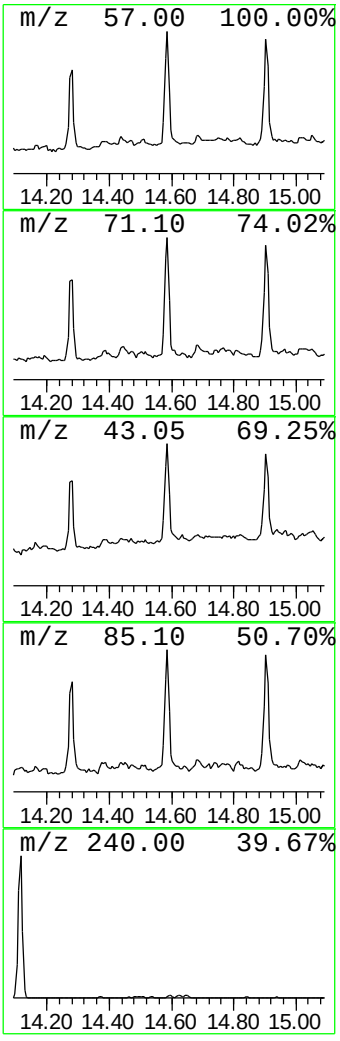
Peak Number 9 Heptadecane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.59	2.39 ng	357704	Chrysene-d12	14.12

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane	240	C17H36	000629-78-7	97
2	Tetracosane	338	C24H50	000646-31-1	81
3	Docosane, 11-butyl-	366	C26H54	013475-76-8	81
4	Hexacosane	366	C26H54	000630-01-3	74
5	Hexatriacontane	507	C36H74	000630-06-8	74





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Data File : BF117749.D
Acq On : 8 Nov 2019 23:25
Operator : JU
Sample : K5668-01 2X
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : HD-01-110619

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110619.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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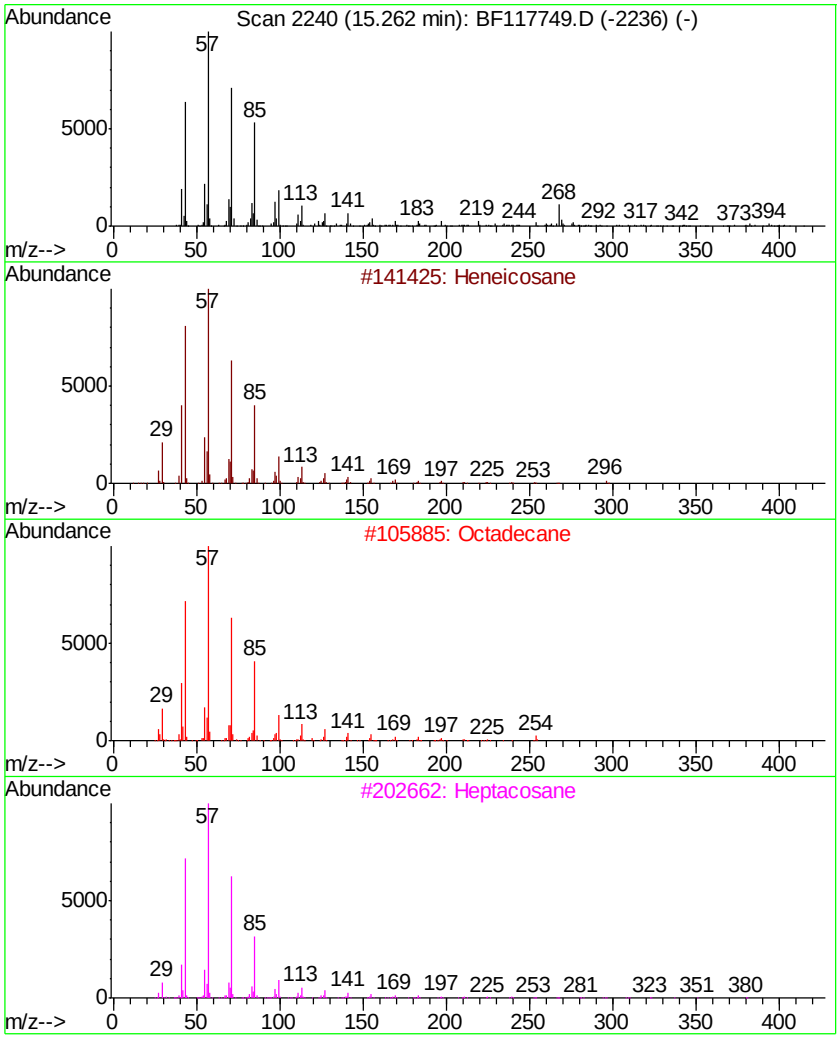
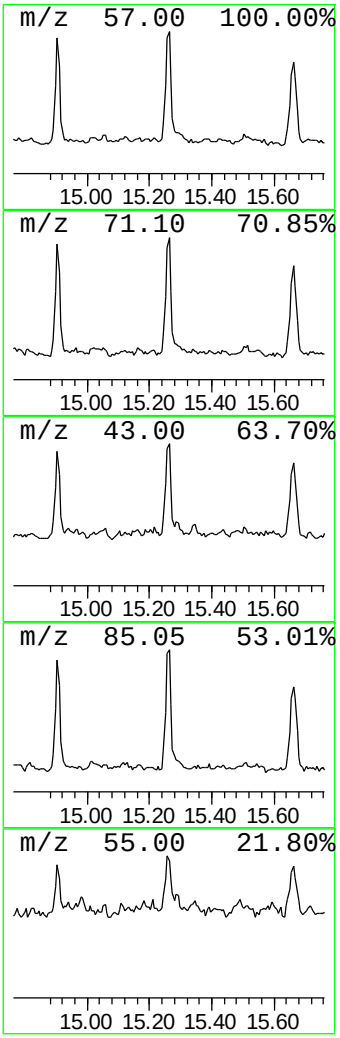
Peak Number 10 Heneicosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.26	3.25 ng	378829	Perylene-d12	15.63

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	96
2	Octadecane	254	C18H38	000593-45-3	96
3	Heptacosane	380	C27H56	000593-49-7	93
4	Eicosane, 10-methyl-	296	C21H44	054833-23-7	91
5	Octacosane	394	C28H58	000630-02-4	90





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF110819\
Data File : BF117749.D
Acq On : 8 Nov 2019 23:25
Operator : JU
Sample : K5668-01 2X
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : HD-01-110619

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110619.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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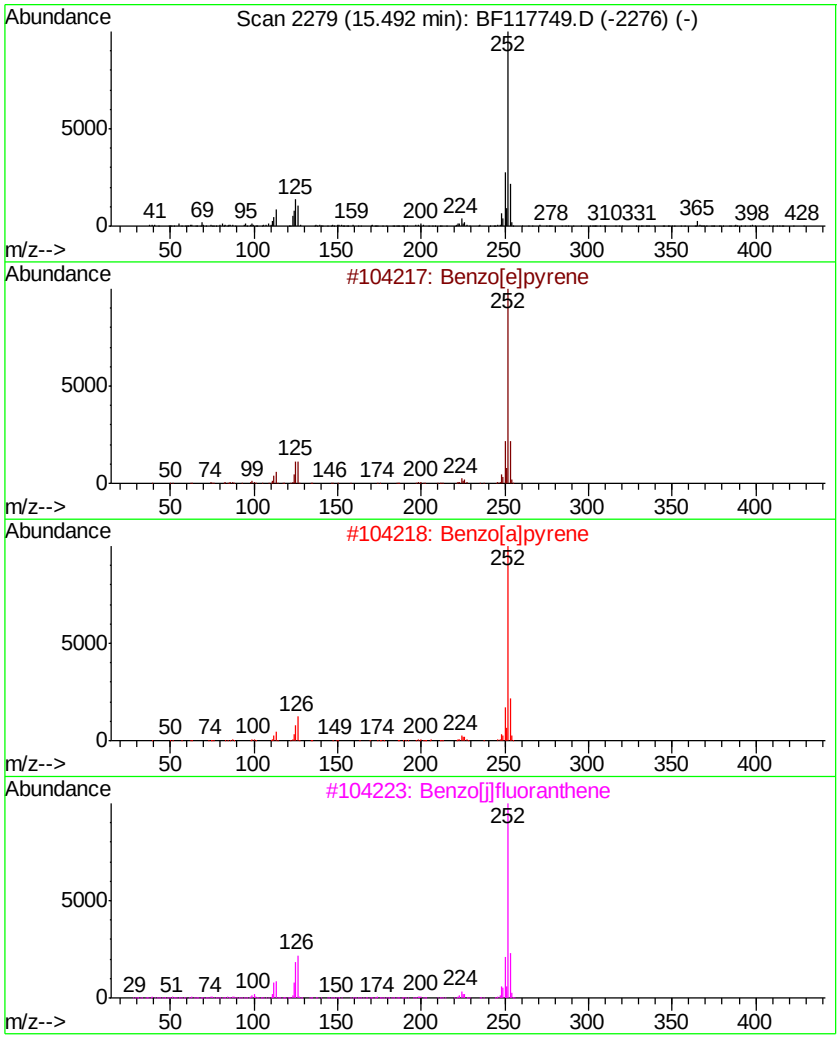
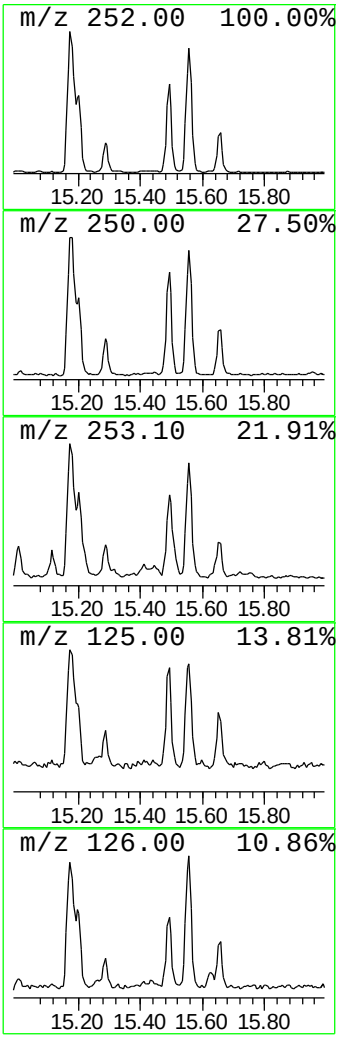
Peak Number 11 Benzo[e]pyrene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.49	4.30 ng	500222	Perylene-d12	15.63

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[e]pyrene	252	C20H12	000192-97-2	98
2	Benzo[a]pyrene	252	C20H12	000050-32-8	98
3	Benzo[j]fluoranthene	252	C20H12	000205-82-3	95
4	Benz[e]acephenanthrylene	252	C20H12	000205-99-2	94
5	Perylene	252	C20H12	000198-55-0	90





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF110819\
Data File : BF117749.D
Acq On : 8 Nov 2019 23:25
Operator : JU
Sample : K5668-01 2X
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : HD-01-110619

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110619.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
Butane, 2-methoxy...	2.20	10.0	ng	1081520	1	6.93	2172460	20.0
2-Pentanone, 4-hy...	5.14	7.2	ng	781643	1	6.93	2172460	20.0
unknown6.69	6.69	36.4	ng	3954570	1	6.93	2172460	20.0
n-Hexadecanoic acid	11.99	5.5	ng	920828	4	11.47	3377010	20.0
9,12-Octadecadien...	12.55	3.3	ng	548346	4	11.47	3377010	20.0
9-Octadecenoic ac...	12.57	5.0	ng	838963	4	11.47	3377010	20.0
Oxalic acid, isob...	13.96	4.8	ng	723323	5	14.12	2991640	20.0
Heptadecane	14.59	2.4	ng	357704	5	14.12	2991640	20.0
Heneicosane	15.26	3.3	ng	378829	6	15.63	2327760	20.0
Benzo[e]pyrene	15.49	4.3	ng	500222	6	15.63	2327760	20.0