LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF030520\
Data File : BF119238.D
Acq On : 6 Mar 2020 3:53
Operator : CG/JU
Sample : L1792-05
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-5

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-BF022020.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	4.934	480	484	498	rVB	225920	330903	9.30%	1.100%
2	5.357	553	556	578	rBV	2473335	2704490	76.04%	8.988%
3	6.381	726	730	748	rBV	2624721	2724289	76.59%	9.054%
4	6.722	785	788	797	rVB	1076224	933005	26.23%	3.101%
5	6.881	811	815	831	rVB	2645347	2419887	68.03%	8.042%
6	7.287	880	884	898	rBV	1768713	1854796	52.15%	6.164%
7	8.004	1002	1006	1015	rBV	1332488	1271704	35.75%	4.226%
8	9.081	1183	1189	1192	rBV	3929770	3556839	100.00%	11.820%
9	9.475	1252	1256	1261	rBV	196575	185451	5.21%	0.616%
10	9.757	1297	1304	1308	rBV	1671960	1493142	41.98%	4.962%
11	9.792	1308	1310	1315	rVB	42037	42927	1.21%	0.143%
12	10.304	1394	1397	1402	rBV	41208	45666	1.28%	0.152%
13	10.551	1435	1439	1449	rBV	2261171	2253327	63.35%	7.488%
14	10.675	1456	1460	1467	rVB2	86669	110406	3.10%	0.367%
15	11.139	1536	1539	1544	rVB	63075	72648	2.04%	0.241%
16	11.239	1553	1556	1559	rBV	1519160	1392456	39.15%	4.628%
17	11.263	1559	1560	1567	rVV	256158	219261	6.16%	0.729%
18	11.322	1567	1570	1573	rVB	54275	53425	1.50%	0.178%
19	11.745	1639	1642	1644	rBV2	44865	46339	1.30%	0.154%
20	11.775	1644	1647	1653	rVV	327099	319099	8.97%	1.060%
21	11.857	1658	1661	1663	rVV	63301	60592	1.70%	0.201%
22	12.292	1732	1735	1738	rBV	51789	51529	1.45%	0.171%
23	12.451	1759	1762	1766	rBV	338635	330996	9.31%	1.100%
24	12.557	1777	1780	1785	rBV3	72366	88135	2.48%	0.293%
25	12.680	1796	1801	1808	rBV	311989	354540	9.97%	1.178%
26	12.822	1821	1825	1828	rBV	3146760	2843810	79.95%	9.451%
27	13.010	1851	1857	1860	rVB	48525	72267	2.03%	0.240%
28	13.080	1866	1869	1872	rBV2	44256	46795	1.32%	0.156%
29	13.116	1872	1875	1882	rVB3	39970	51215	1.44%	0.170%
30	13.745	1976	1982	1990	rBV4	119339	283697	7.98%	0.943%
31	13.880	1998	2005	2008	rBV2	1003988	1067990	30.03%	3.549%
32	14.039	2029	2032	2036	rVB2	56860	62494	1.76%	0.208%
33	14.339	2080	2083	2086	rBV	110607	100340	2.82%	0.333%
34	14.633	2131	2133	2138	rVV	85543	84448	2.37%	0.281%

LSC Area Percent Report

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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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Peak separation: 5

Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF022020.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	14.704	2142	2145	2150	rVB	295180	308579	8.68%	1.026%
36	14.904	2176	2179	2182	rBV	119746	161675	4.55%	0.537%
37	14.951	2184	2187	2194	rVB	153221	188187	5.29%	0.625%
38	15.192	2224	2228	2234	rVB	105865	138557	3.90%	0.460%
39	15.251	2234	2238	2242	rBV	108924	134754	3.79%	0.448%
40	15.304	2243	2247	2262	rVB	851894	1157621	32.55%	3.847%
41	15.710	2312	2316	2323	rVB	94382	139964	3.94%	0.465%
42	16.174	2392	2395	2398	rBV3	31788	41089	1.16%	0.137%
43	16.715	2483	2487	2496	rBV3	73958	155251	4.36%	0.516%
44	17.139	2554	2559	2567	rVB	60164	135999	3.82%	0.452%

Sum of corrected areas: 30090584

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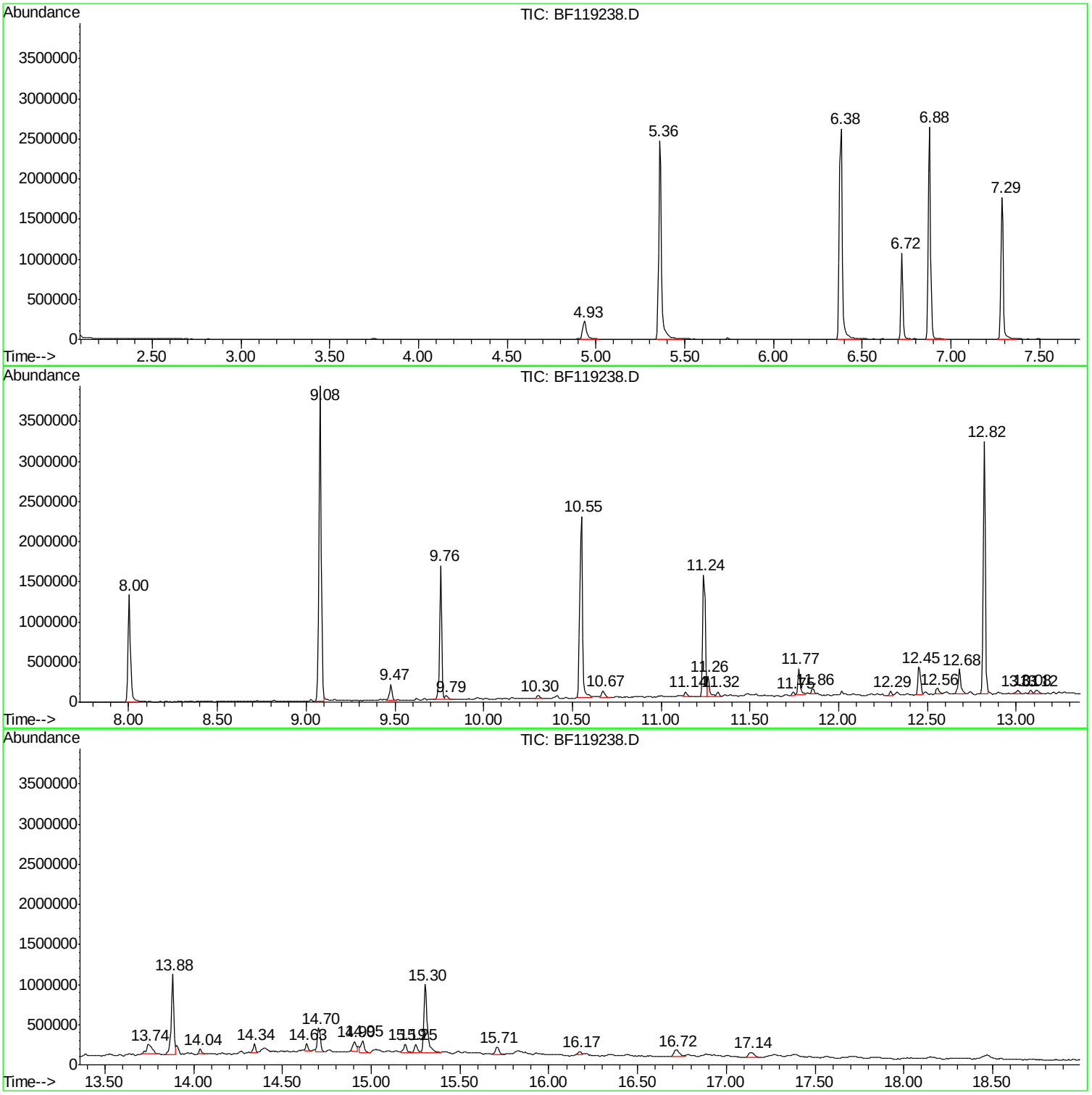
BNA_F
ClientSampleId :
TP-5

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF022020.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 : BF119238.D
Acq On : 6 Mar 2020 3:53
Operator : CG/JU
Sample : L1792-05
Misc :
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Instrument : BNA_F
ClientSampleId : TP-5

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF022020.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

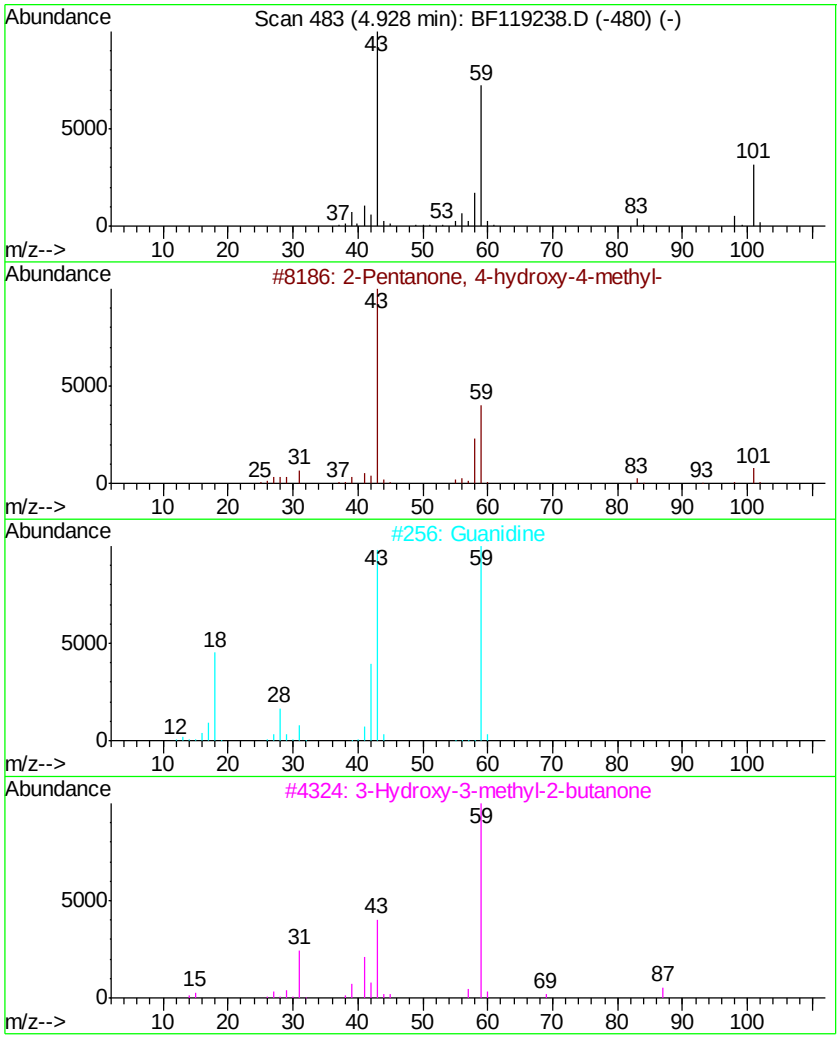
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

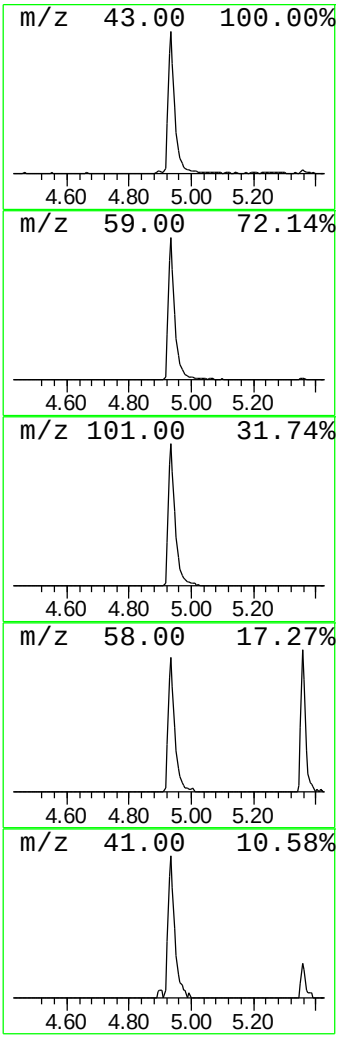
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.93	7.09 ng	330903	1,4-Dichlorobenzene-d4	6.72

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2	Guanidine	59	CH5N3	000113-00-8	50
3	3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	38
4	(+-)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	35
5	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	28





Library Search Compound Report

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Operator : CG/JU
Sample : L1792-05
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-5

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF022020.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
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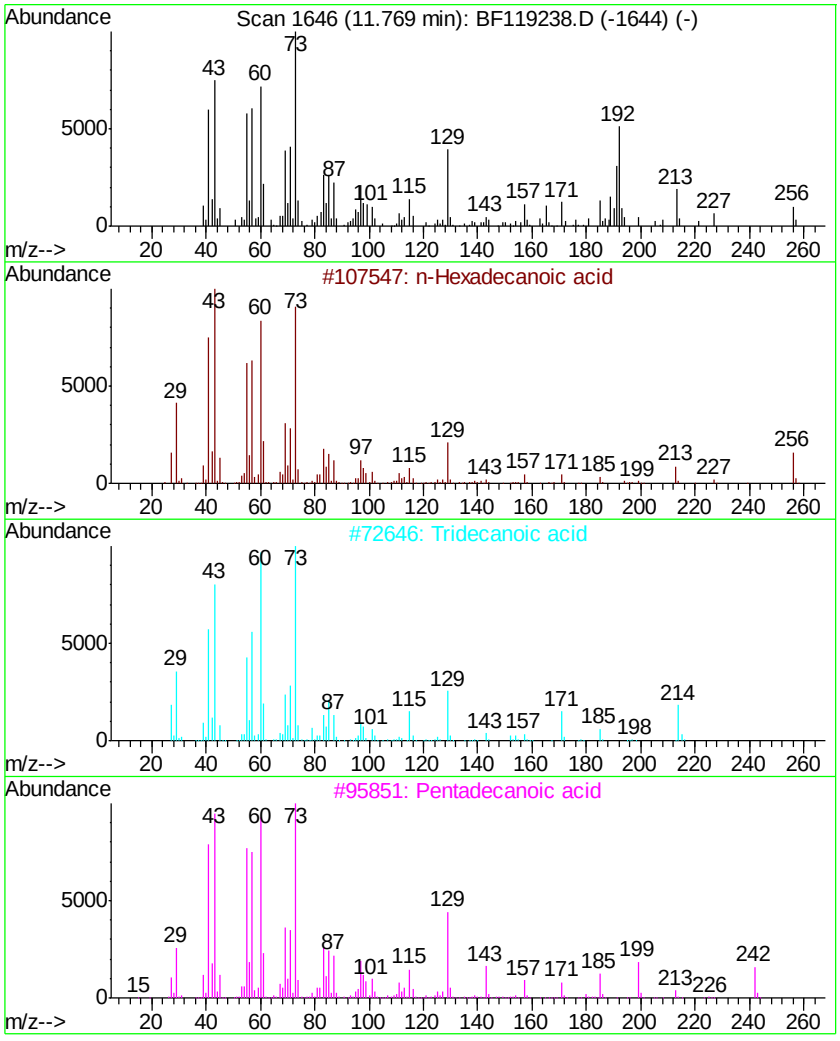
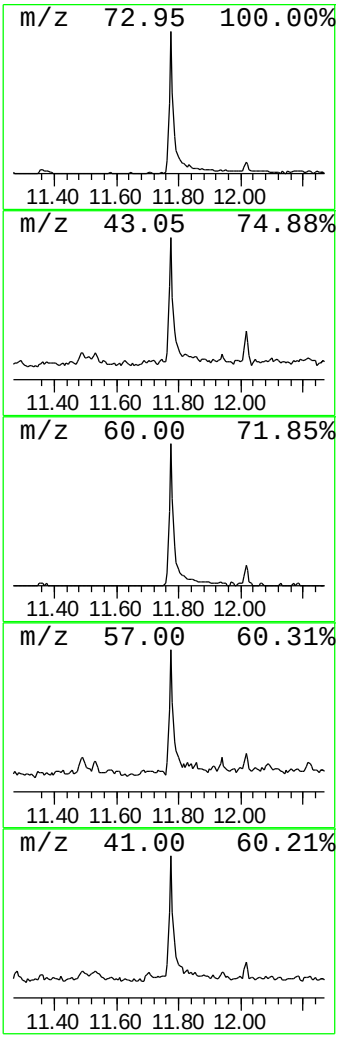
Peak Number 3 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.77	4.58 ng	319099	Phenanthrene-d10	11.24

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	96
2	Tridecanoic acid	214	C13H26O2	000638-53-9	78
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	60
4	n-Decanoic acid	172	C10H20O2	000334-48-5	50
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	47





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Instrument : BNA_F
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF022020.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
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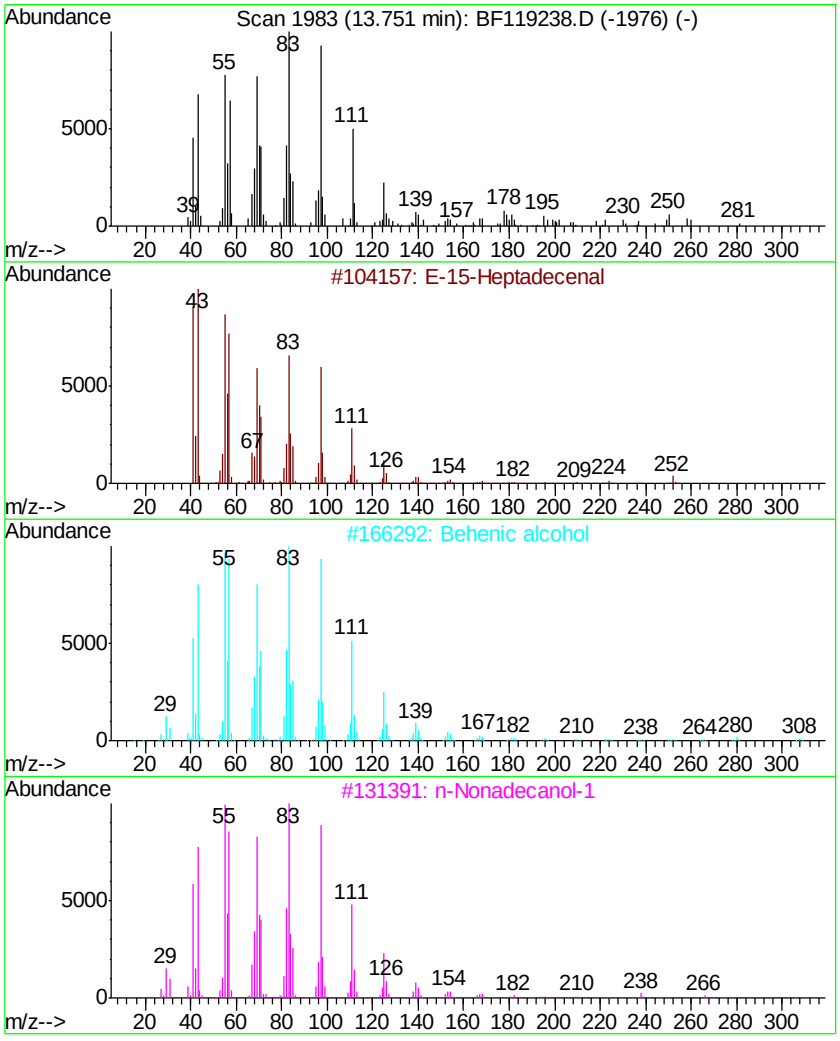
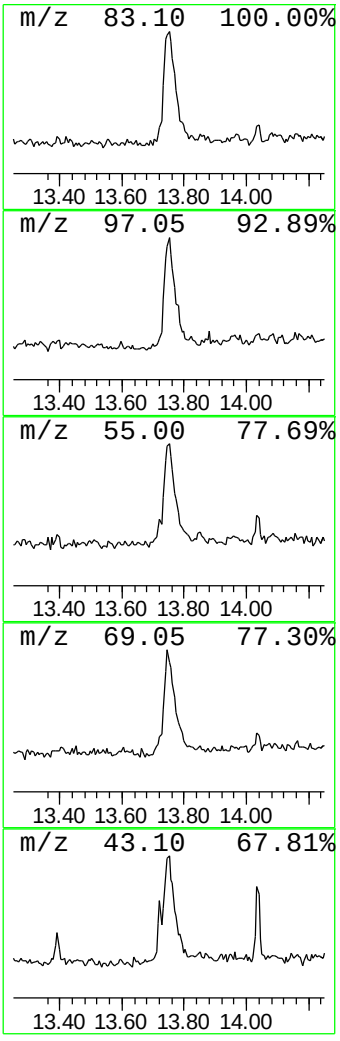
Peak Number 4 E-15-Heptadecenal Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.75	5.31 ng	283697	Chrysene-d12	13.88

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	E-15-Heptadecenal	252	C17H32O	1000130-97-9	95
2	Behenic alcohol	326	C22H46O	000661-19-8	93
3	n-Nonadecanol-1	284	C19H40O	001454-84-8	93
4	Cyclohexadecane	224	C16H32	000295-65-8	93
5	Cyclopentadecane	210	C15H30	000295-48-7	87





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Instrument : BNA_F
ClientSampleId : TP-5

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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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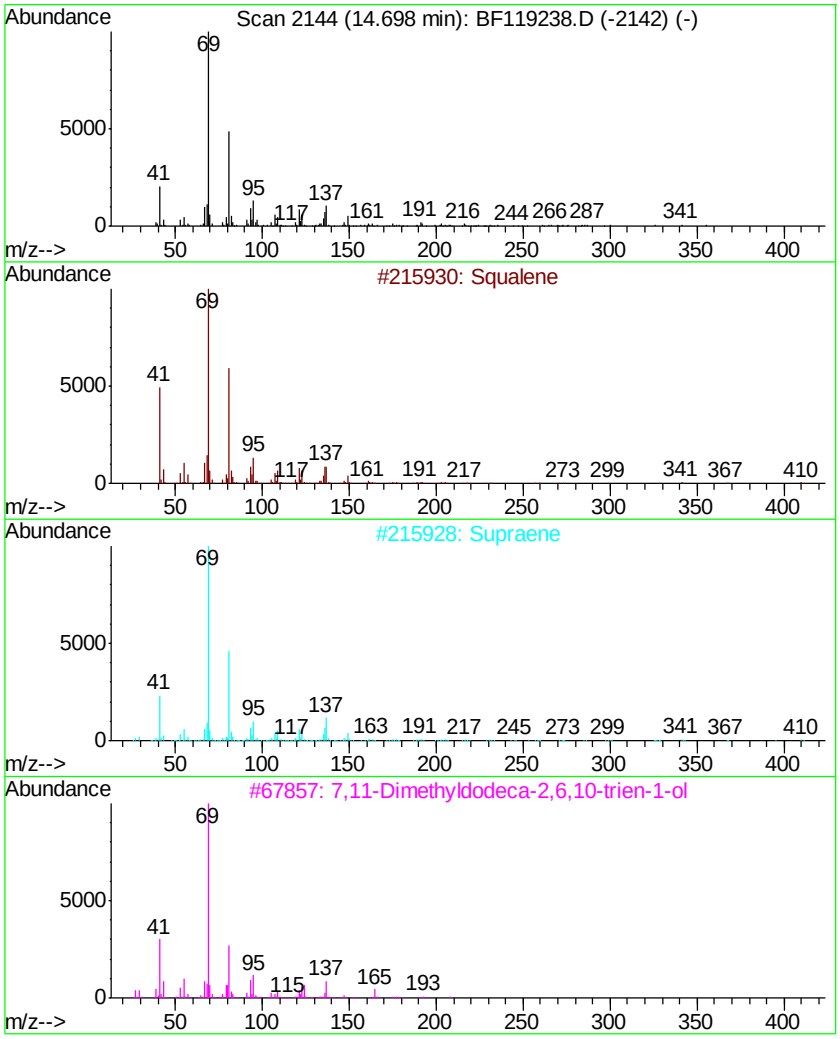
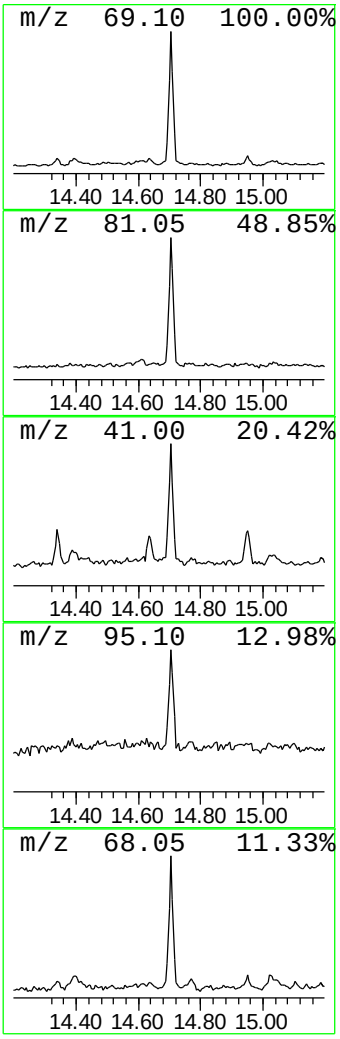
Peak Number 5 Squalene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.70	5.33 ng	308579	Perylene-d12	15.30

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Squalene	410	C30H50	000111-02-4	91
2	Supraene	410	C30H50	007683-64-9	91
3	7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	74
4	2,6,10,14-Hexadecatetraenoic aci...	332	C22H36O2	024035-35-6	72
5	1,5,9-Decatriene, 2,3,5,8-tetram...	192	C14H24	230646-72-7	64





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Misc :
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Instrument : BNA_F
ClientSampleId : TP-5

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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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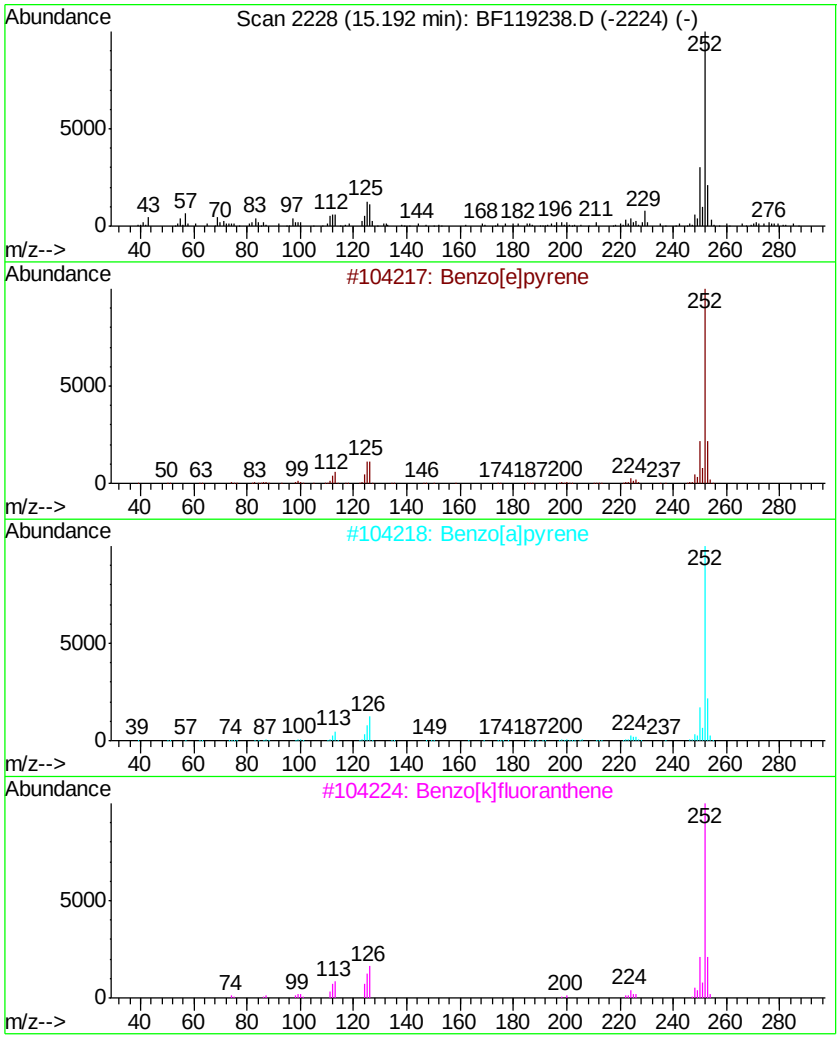
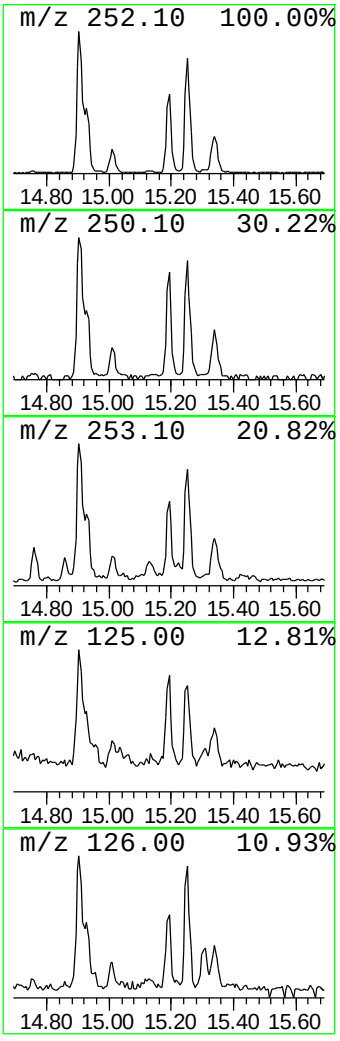
Peak Number 6 Benzo[e]pyrene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.19	2.39 ng	138557	Perylene-d12	15.30

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[e]pyrene	252	C20H12	000192-97-2	97
2	Benzo[a]pyrene	252	C20H12	000050-32-8	96
3	Benzo[k]fluoranthene	252	C20H12	000207-08-9	95
4	Benz[e]acephenanthrylene	252	C20H12	000205-99-2	95
5	Perylene	252	C20H12	000198-55-0	90





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

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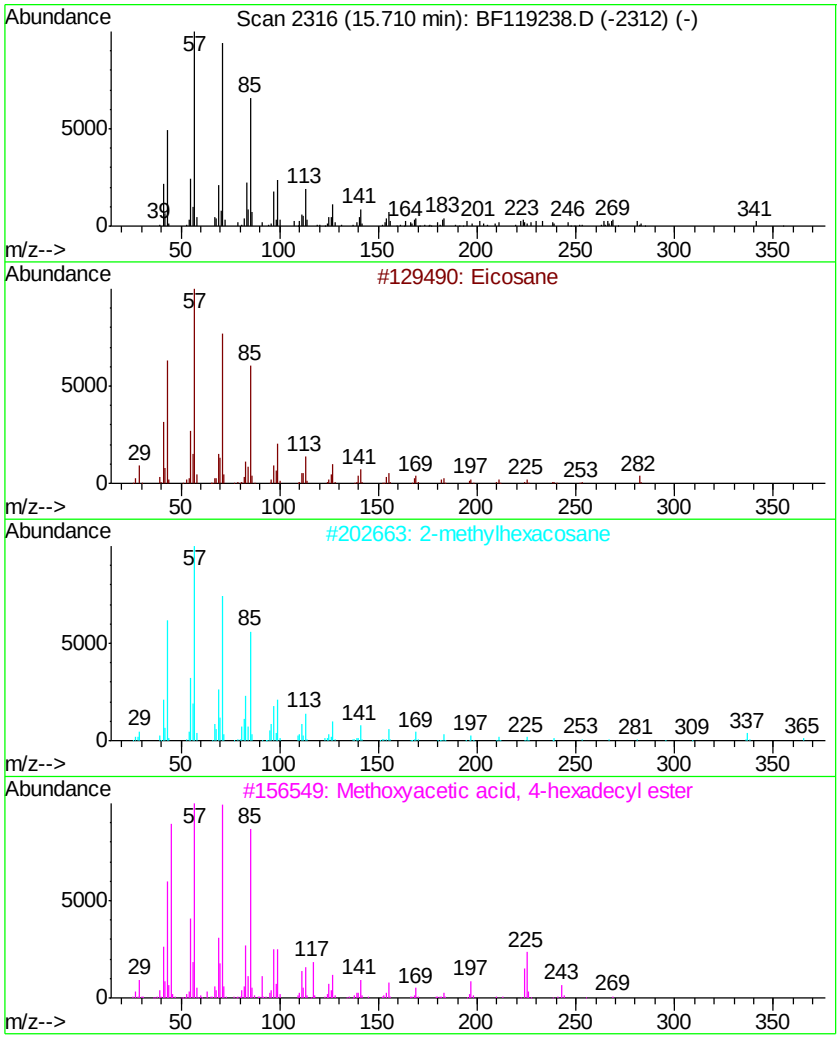
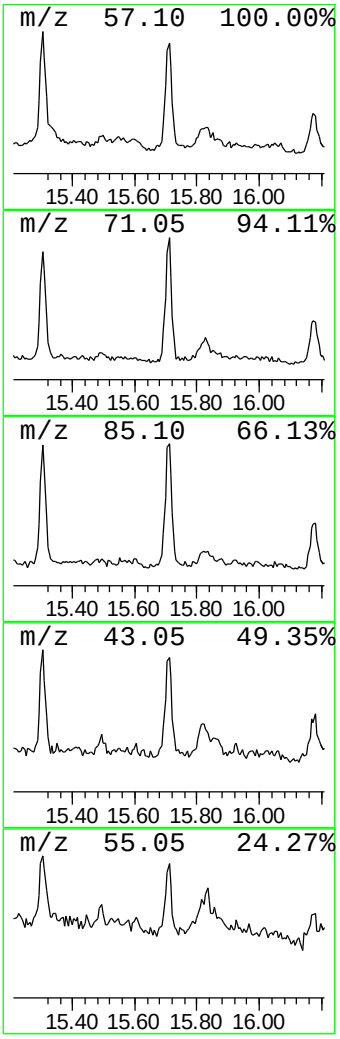
Peak Number 7 Eicosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.71	2.42 ng	139964	Perylene-d12	15.30

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	87
2	2-methylhexacosane	380	C27H56	1000376-72-7	87
3	Methoxyacetic acid, 4-hexadecyl ...	314	C19H38O3	1000282-99-0	86
4	5-Butyl-5-ethylheptadecane	324	C23H48	1000360-43-0	86
5	Tetracosane	338	C24H50	000646-31-1	83





Tentatively Identified Compound (LSC) summary

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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
2-Pentanone, 4-hy...	4.93	7.1	ng	330903	1	6.72	933005	20.0
n-Hexadecanoic acid	11.77	4.6	ng	319099	4	11.24	1392460	20.0
E-15-Heptadecenal	13.75	5.3	ng	283697	5	13.88	1067990	20.0
Squalene	14.70	5.3	ng	308579	6	15.30	1157620	20.0
Benzo[e]pyrene	15.19	2.4	ng	138557	6	15.30	1157620	20.0
Eicosane	15.71	2.4	ng	139964	6	15.30	1157620	20.0