LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102620\
Data File : BF122124.D
Acq On : 26 Oct 2020 19:41
Operator : JU/CG
Sample : L4436-05
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 34B

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-BF101220.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF122124.D\data.ms

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	499	rBV	25692	42952	1.45%	0.187%
2	5.340	549	553	582	rBV	2297949	2553327	86.40%	11.139%
3	6.369	724	728	755	rBV	2365945	2629080	88.97%	11.470%
4	6.569	760	762	781	rVB	31996	72099	2.44%	0.315%
5	6.710	783	786	795	rVB	708140	655204	22.17%	2.858%
6	7.287	879	884	896	rBV	1735085	1804834	61.07%	7.874%
7	7.998	1001	1005	1019	rVB	910053	883337	29.89%	3.854%
8	9.069	1182	1187	1191	rBV	3146114	2955116	100.00%	12.892%
9	9.469	1251	1255	1263	rBV	393039	343716	11.63%	1.500%
10	9.745	1298	1302	1306	rBV	1208972	1006686	34.07%	4.392%
11	10.539	1433	1437	1446	rBV	1868783	1646144	55.70%	7.182%
12	11.233	1551	1555	1557	rBV	1092824	967647	32.74%	4.221%
13	11.257	1557	1559	1562	rVB	184526	149038	5.04%	0.650%
14	11.733	1636	1640	1642	rBV2	48305	51282	1.74%	0.224%
15	11.763	1642	1645	1652	rVV2	133249	136615	4.62%	0.596%
16	11.845	1656	1659	1662	rBV	49085	48939	1.66%	0.214%
17	12.445	1758	1761	1765	rBV	311663	259347	8.78%	1.131%
18	12.545	1775	1778	1785	rBV2	58882	85147	2.88%	0.371%
19	12.674	1795	1800	1804	rBV	269096	275147	9.31%	1.200%
20	12.816	1819	1824	1827	rBV	2850911	2539299	85.93%	11.078%
21	12.892	1834	1837	1842	rBV3	20756	37437	1.27%	0.163%
22	12.945	1844	1846	1849	rVV	43495	40976	1.39%	0.179%
23	13.039	1859	1862	1865	rBV	42573	43808	1.48%	0.191%
24	13.110	1870	1874	1881	rVB3	33299	41310	1.40%	0.180%
25	13.310	1905	1908	1911	rVB	40916	35238	1.19%	0.154%
26	13.380	1917	1920	1923	rBV3	34078	40550	1.37%	0.177%
27	13.716	1973	1977	1986	rVB2	212582	432108	14.62%	1.885%
28	13.845	1995	1999	2000	rBV	80676	77063	2.61%	0.336%
29	13.874	2000	2004	2007	rVV2	840458	864518	29.25%	3.772%
30	13.898	2007	2008	2016	rVB	128511	117829	3.99%	0.514%
31	14.027	2027	2030	2033	rBV2	29607	33119	1.12%	0.144%
32	14.327	2078	2081	2084	rBV2	57937	70837	2.40%	0.309%
33	14.363	2084	2087	2090	rVV3	33391	49520	1.68%	0.216%
34	14.486	2105	2108	2112	rBV	204678	190170	6.44%	0.830%
35	14.763	2152	2155	2159	rVB2	93861	94131	3.19%	0.411%
36	14.898	2175	2178	2181	rBV	104115	136118	4.61%	0.594%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102620\
Data File : BF122124.D
Acq On : 26 Oct 2020 19:41
Operator : JU/CG
Sample : L4436-05
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 34B

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-BF101220.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	15.004	2190	2196	2203	rBV4	70661	171444	5.80%	0.748%
38	15.186	2224	2227	2230	rBV	82733	104326	3.53%	0.455%
39	15.245	2235	2237	2242	rVV	99474	121514	4.11%	0.530%
40	15.304	2243	2247	2251	rVV	570690	668921	22.64%	2.918%
41	15.486	2275	2278	2283	rBV3	36665	48350	1.64%	0.211%
42	15.698	2311	2314	2319	rVB	66341	84226	2.85%	0.367%
43	15.786	2324	2329	2337	rVV10	37287	117892	3.99%	0.514%
44	16.710	2482	2486	2496	rVB	70644	140522	4.76%	0.613%
45	17.139	2555	2559	2566	rVB2	30591	55034	1.86%	0.240%

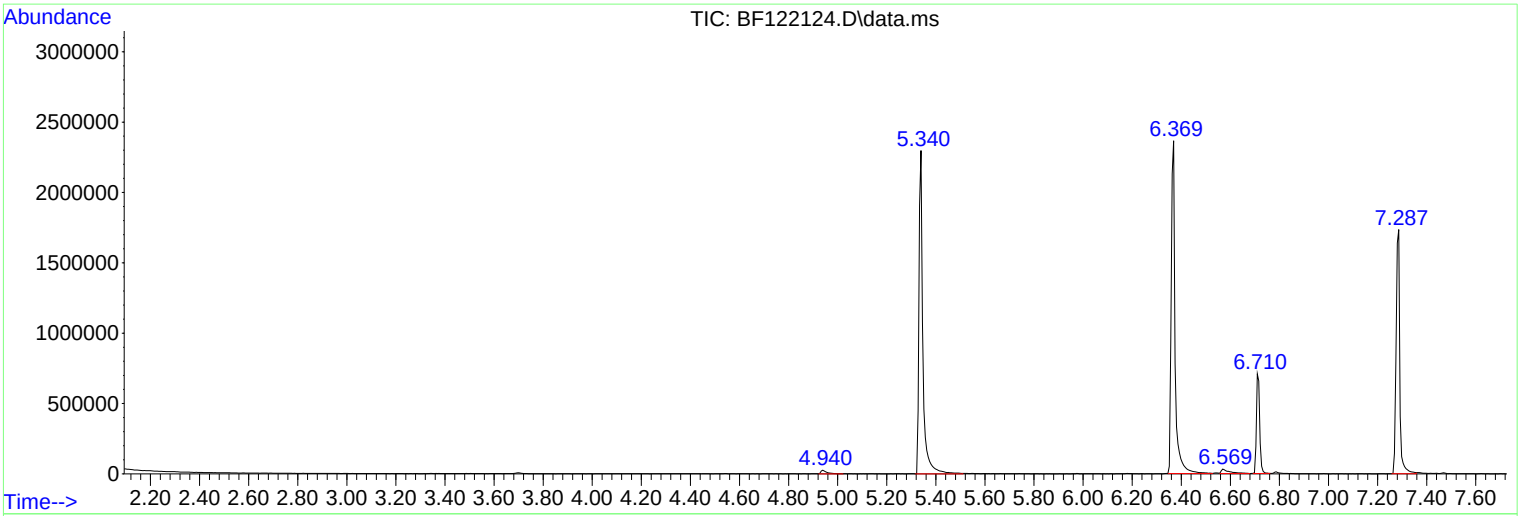
Sum of corrected areas: 22921917

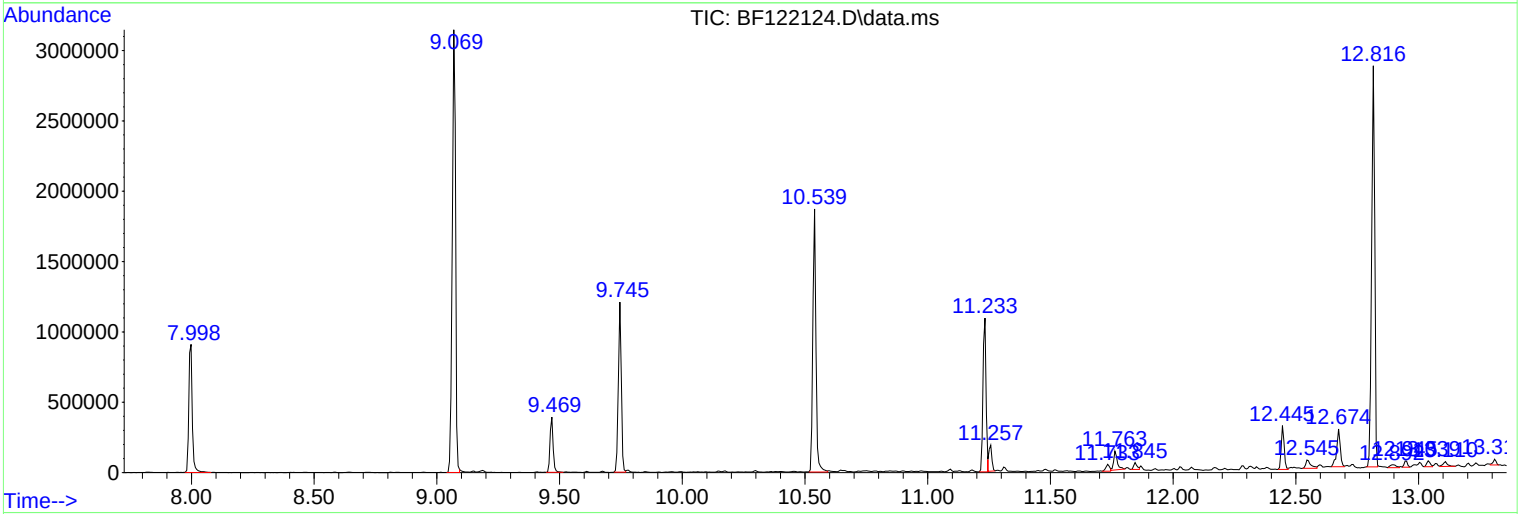
Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102620\
Data File : BF122124.D
Acq On : 26 Oct 2020 19:41
Operator : JU/CG
Sample : L4436-05
Misc :
ALS Vial : 10 Sample Multiplier: 1

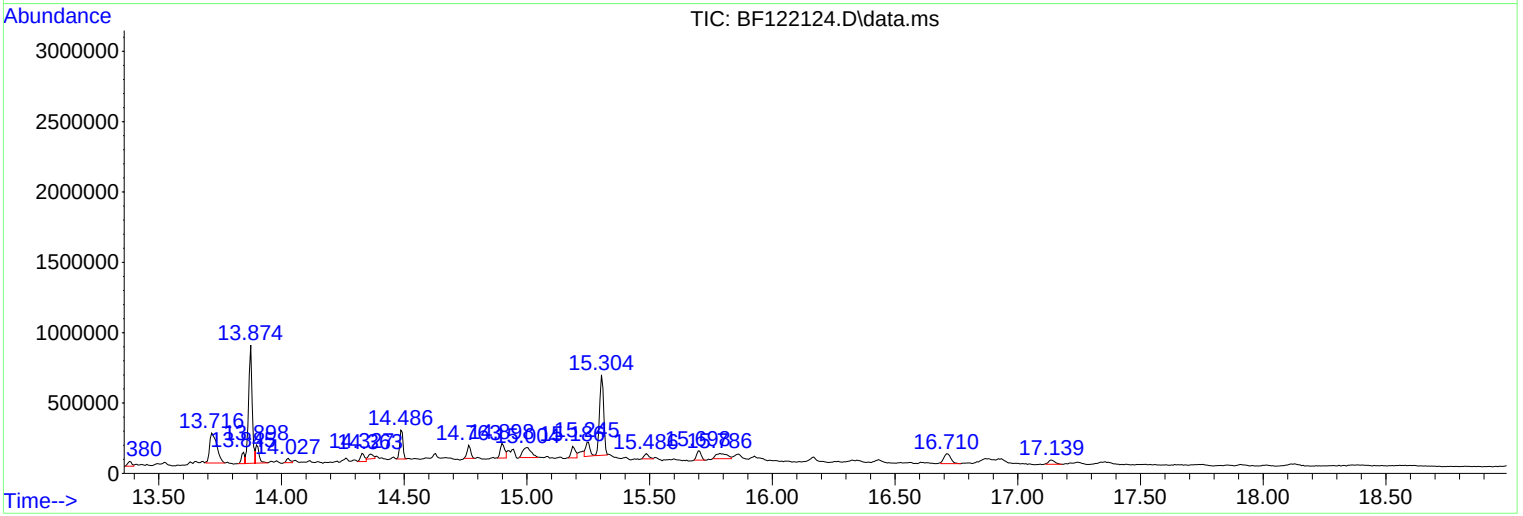
Instrument :
BNA_F
ClientSampleId :
34B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101220.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\BF102620\
Data File : BF122124.D
Acq On : 26 Oct 2020 19:41
Operator : JU/CG
Sample : L4436-05
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 34B

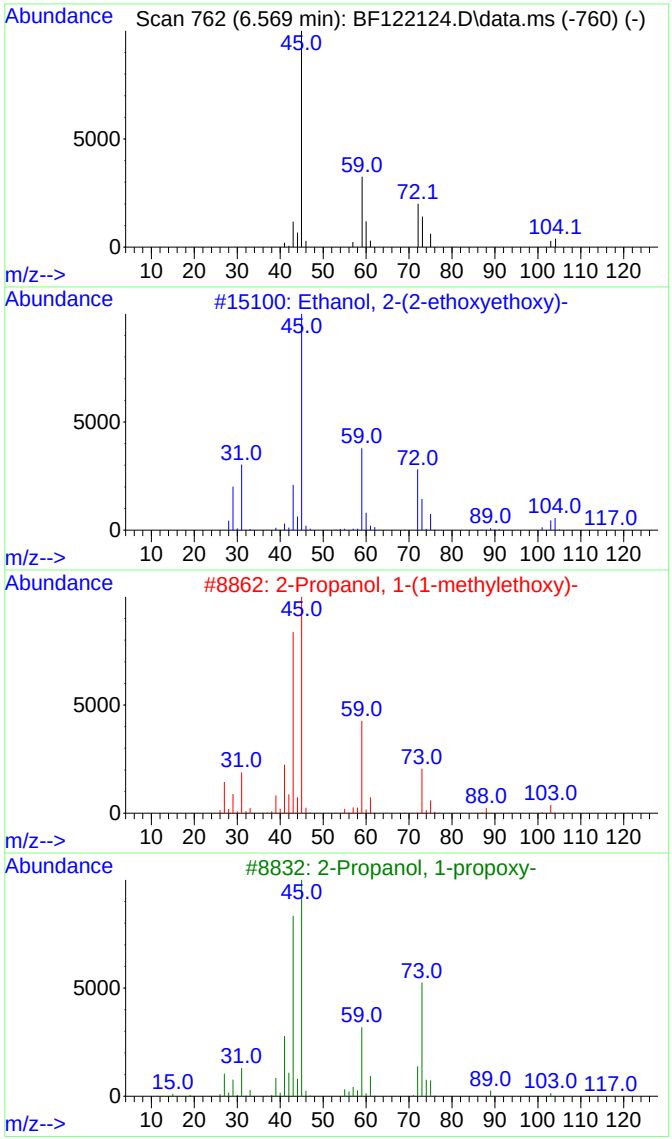
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101220.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

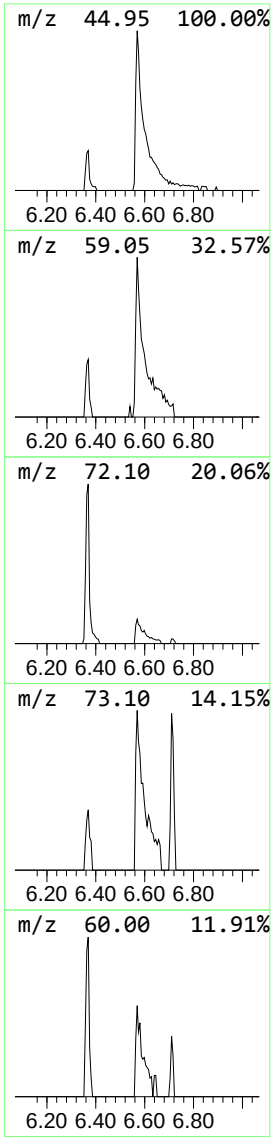
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 Ethanol, 2-(2-ethoxyethoxy)- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.569	2.20 ng	72099	1,4-Dichlorobenzene-d4	6.710

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(2-ethoxyethoxy)-	134	C6H14O3	000111-90-0	83
2	2-Propanol, 1-(1-methylethoxy)-	118	C6H14O2	003944-36-3	45
3	2-Propanol, 1-propoxy-	118	C6H14O2	001569-01-3	39
4	2-Hydroxyethyl vinyl sulfide	104	C4H8OS	003090-56-0	9
5	Acetic acid, hydroxy-, ethyl ester	104	C4H8O3	000623-50-7	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102620\
Data File : BF122124.D
Acq On : 26 Oct 2020 19:41
Operator : JU/CG
Sample : L4436-05
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 34B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101220.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

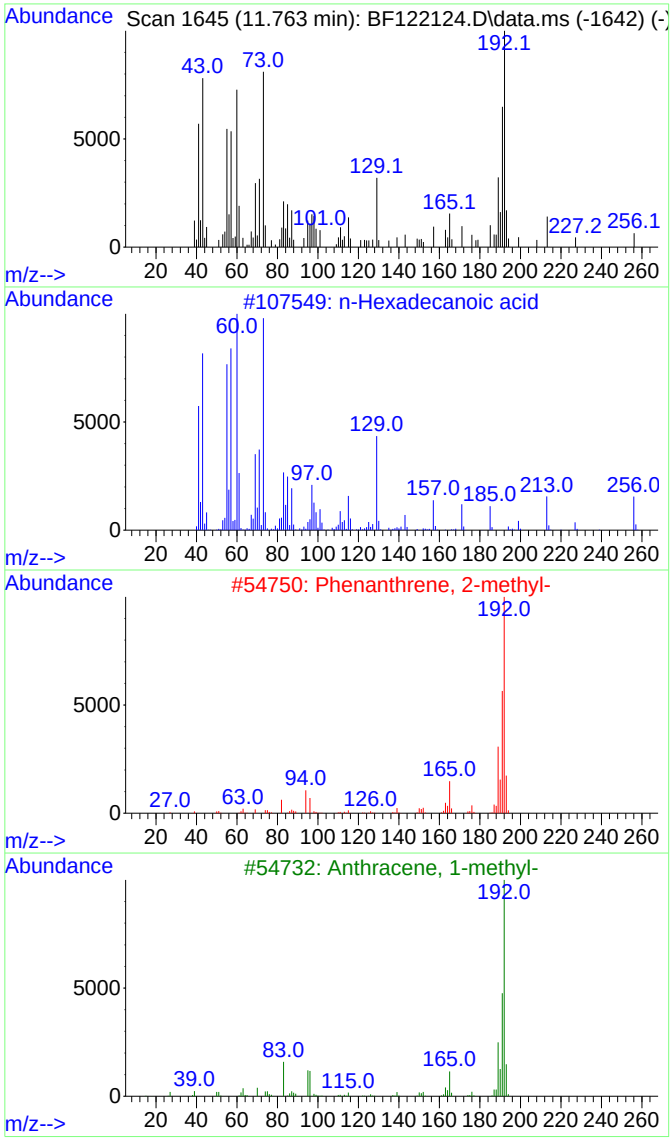
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

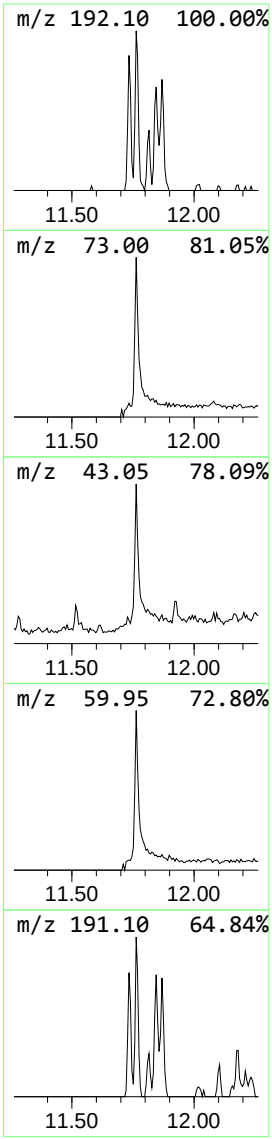
****

Peak Number 2 n-Hexadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.763	2.82 ng	136615	Phenanthrene-d10	11.233

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	96
2	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	94
3	Anthracene, 1-methyl-	192	C15H12	000610-48-0	93
4	Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	89
5	Anthracene, 2-methyl-	192	C15H12	000613-12-7	83





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102620\
Data File : BF122124.D
Acq On : 26 Oct 2020 19:41
Operator : JU/CG
Sample : L4436-05
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 34B

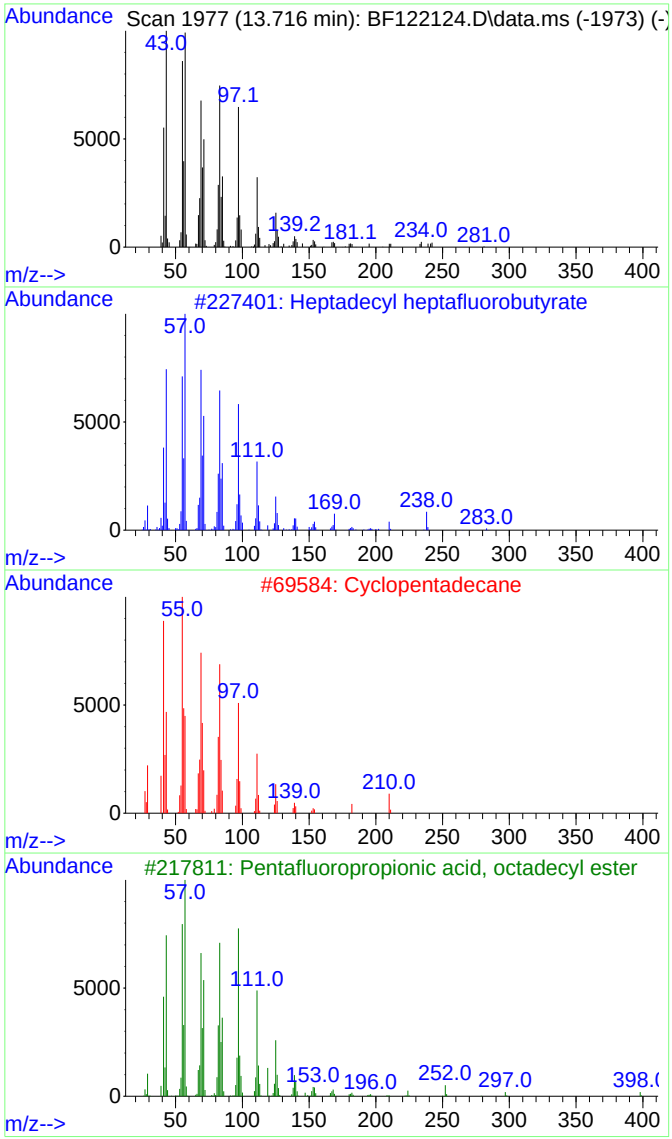
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101220.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

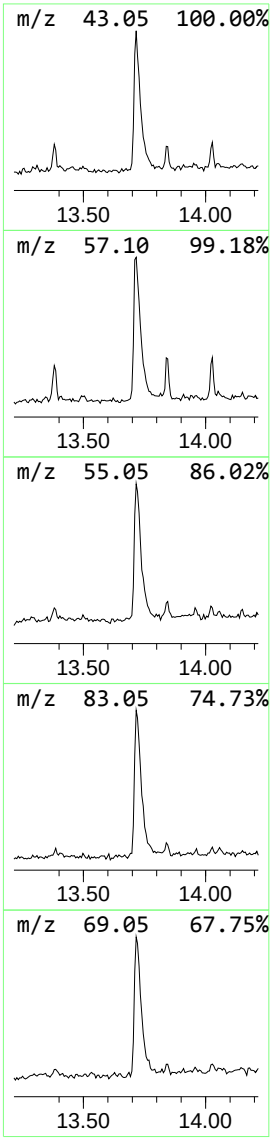
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Heptadecyl heptafluorobutyrate Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.716	10.00 ng	432108	Chrysene-d12	13.874

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94
2	Cyclopentadecane	210	C15H30	000295-48-7	93
3	Pentafluoropropionic acid, octad...	416	C21H37F5O2	959261-25-7	91
4	Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	91
5	Pentafluoropropionic acid, tetra...	360	C17H29F5O2	006222-06-6	91





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102620\
Data File : BF122124.D
Acq On : 26 Oct 2020 19:41
Operator : JU/CG
Sample : L4436-05
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 34B

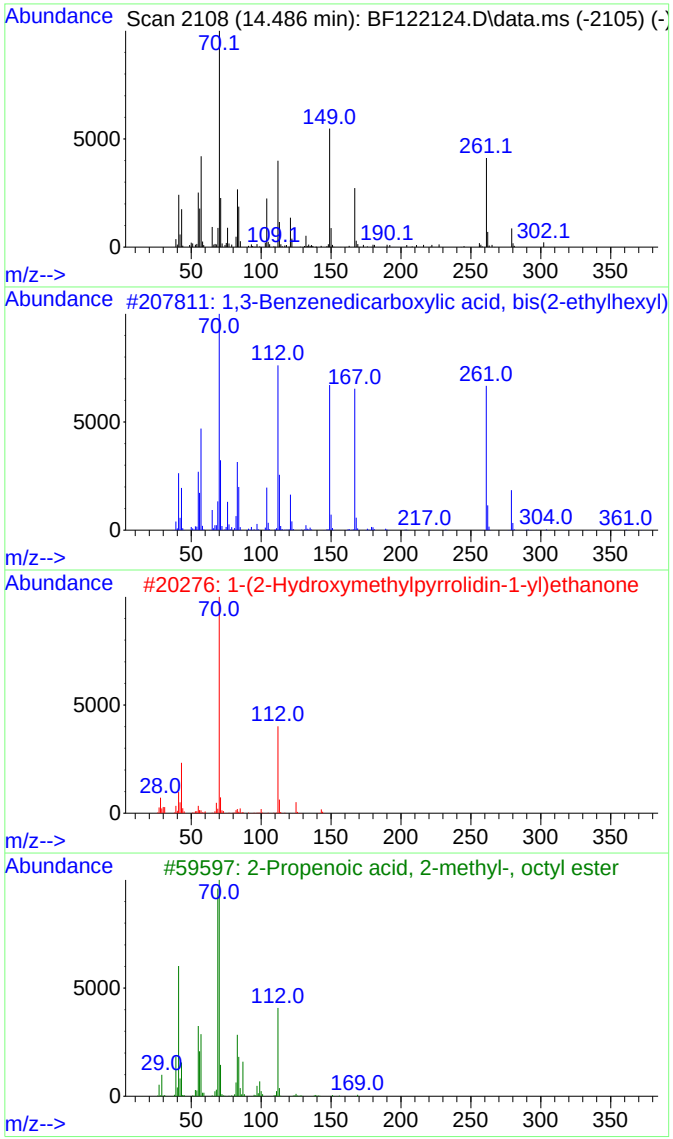
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101220.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

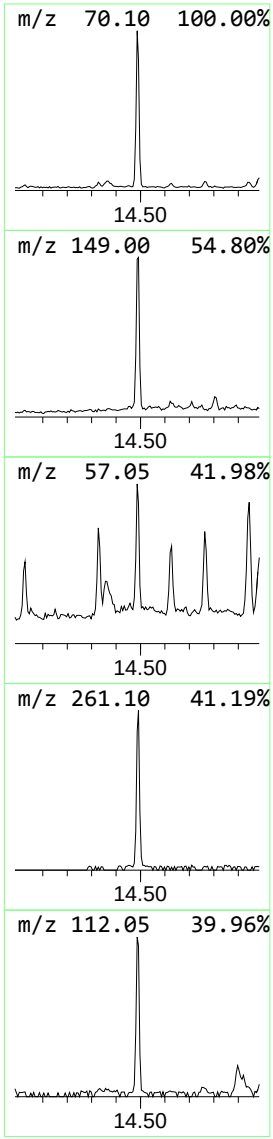
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 1,3-Benzenedicarboxylic aci... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.486	4.40 ng	190170	Chrysene-d12	13.874

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3-Benzenedicarboxylic acid, bi...	390	C24H38O4	000137-89-3	58
2	1-(2-Hydroxymethylpyrrolidin-1-y...	143	C7H13NO2	1000192-83-2	38
3	2-Propenoic acid, 2-methyl-, oct...	198	C12H22O2	002157-01-9	25
4	Di-n-octyl phthalate	390	C24H38O4	000117-84-0	22
5	Cyclohexanamine, N-methyl-	113	C7H15N	000100-60-7	22





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102620\
Data File : BF122124.D
Acq On : 26 Oct 2020 19:41
Operator : JU/CG
Sample : L4436-05
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 34B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101220.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

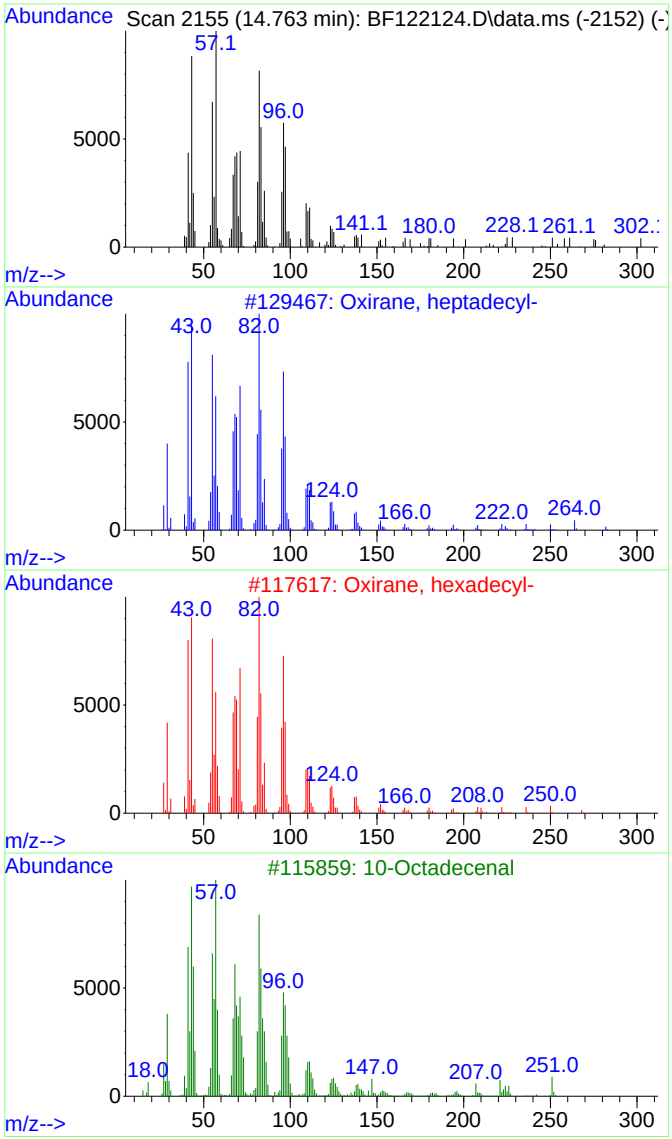
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

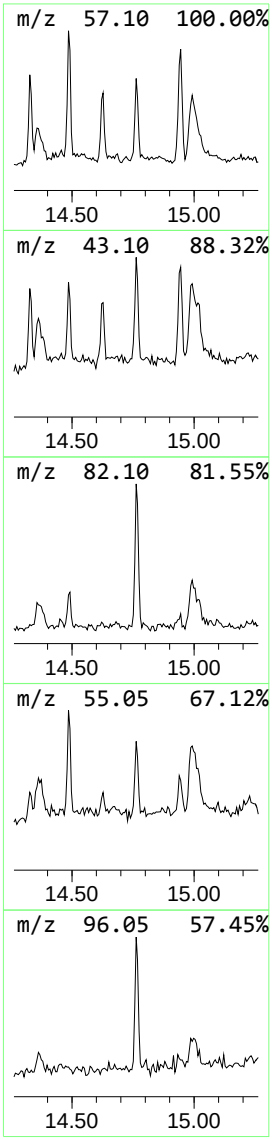
****

Peak Number 5 Oxirane, heptadecyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.763	2.81 ng	94131	Perylene-d12	15.304

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oxirane, heptadecyl-	282	C19H38O	067860-04-2	83
2	Oxirane, hexadecyl-	268	C18H36O	007390-81-0	74
3	10-Octadecenal	266	C18H34O	056554-92-8	72
4	1,19-Eicosadiene	278	C20H38	014811-95-1	68
5	Octadecanal	268	C18H36O	000638-66-4	58





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102620\
Data File : BF122124.D
Acq On : 26 Oct 2020 19:41
Operator : JU/CG
Sample : L4436-05
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 34B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101220.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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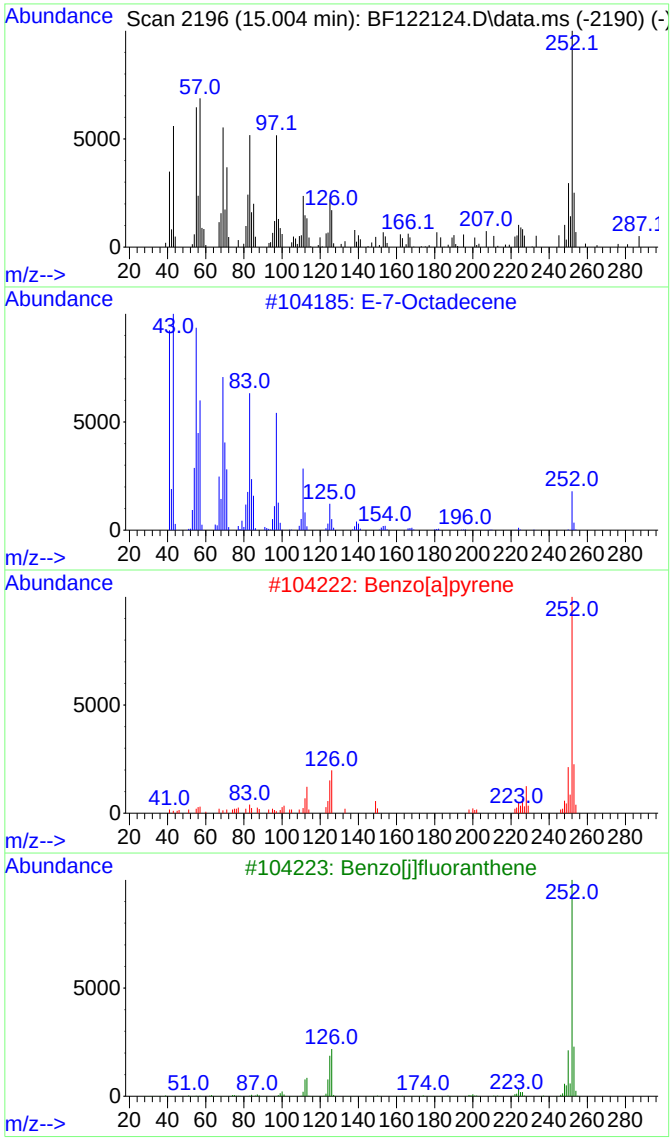
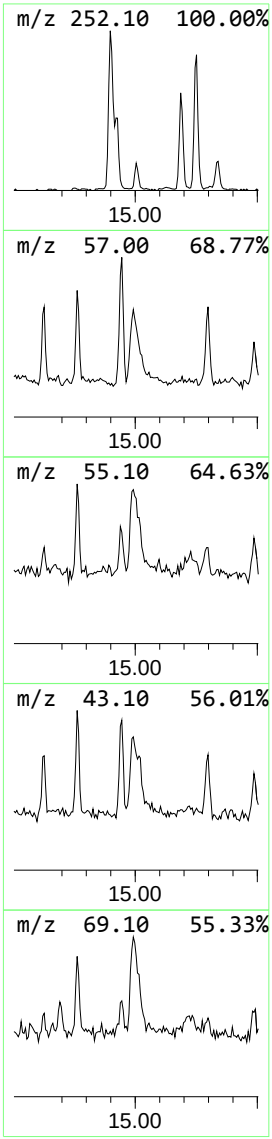
Peak Number 6 E-7-Octadecene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.004	5.13 ng	171444	Perylene-d12	15.304

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	E-7-Octadecene	252	C18H36	1000130-92-0	58
2	Benzo[a]pyrene	252	C20H12	000050-32-8	50
3	Benzo[j]fluoranthene	252	C20H12	000205-82-3	43
4	Pentafluoropropionic acid, octad...	416	C21H37F5O2	959261-25-7	42
5	Heptafluorobutyric acid, n-octad...	466	C22H37F7O2	000400-57-7	38





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102620\
Data File : BF122124.D
Acq On : 26 Oct 2020 19:41
Operator : JU/CG
Sample : L4436-05
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 34B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101220.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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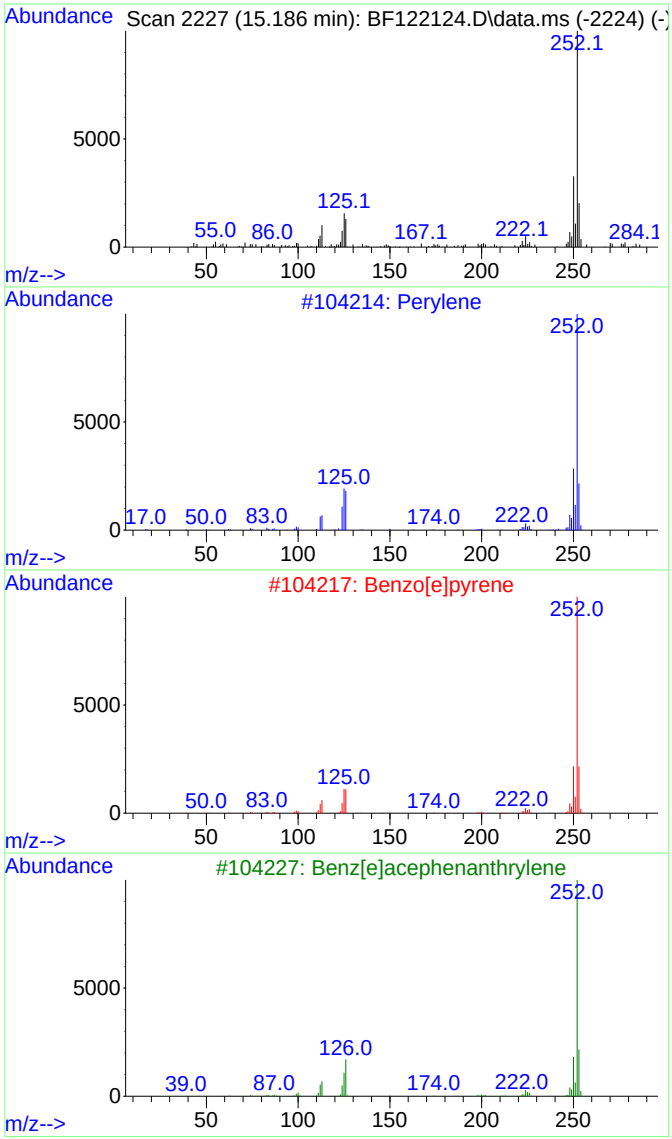
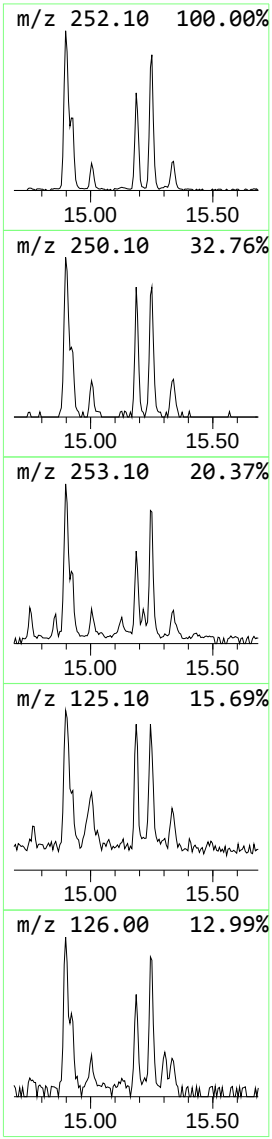
Peak Number 7 Perylene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.186	3.12 ng	104326	Perylene-d12	15.304

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Perylene	252	C20H12	000198-55-0	96
2	Benzo[e]pyrene	252	C20H12	000192-97-2	96
3	Benz[e]acephenanthrylene	252	C20H12	000205-99-2	93
4	Benzo[a]pyrene	252	C20H12	000050-32-8	93
5	Benzo[k]fluoranthene	252	C20H12	000207-08-9	89





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102620\
Data File : BF122124.D
Acq On : 26 Oct 2020 19:41
Operator : JU/CG
Sample : L4436-05
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 34B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101220.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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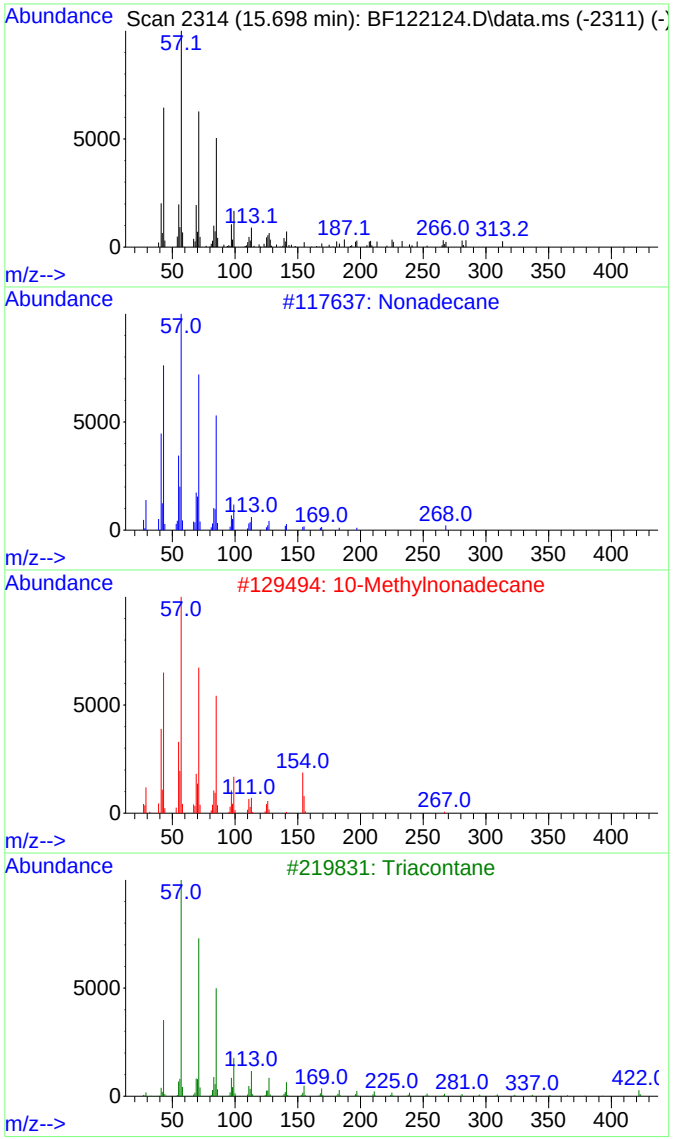
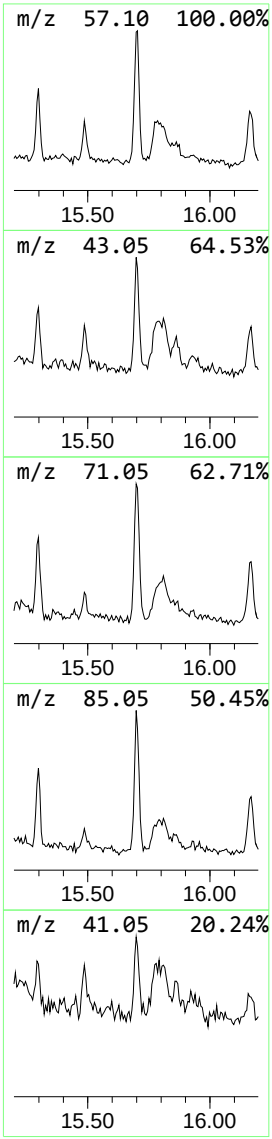
Peak Number 8 Nonadecane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.698	2.52 ng	84226	Perylene-d12	15.304

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonadecane	268	C19H40	000629-92-5	94
2	10-Methylnonadecane	282	C20H42	056862-62-5	86
3	Triacontane	422	C30H62	000638-68-6	86
4	Heneicosane	296	C21H44	000629-94-7	83
5	Octadecane, 1-iodo-	380	C18H37I	000629-93-6	80





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Acq On : 26 Oct 2020 19:41
Operator : JU/CG
Sample : L4436-05
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 34B

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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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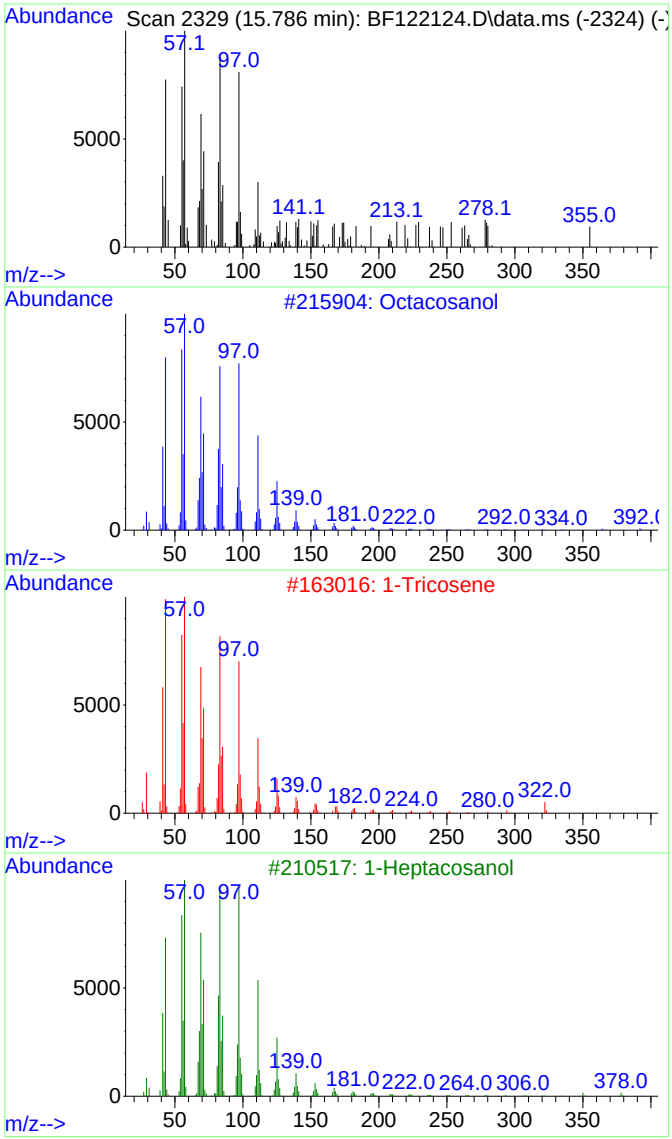
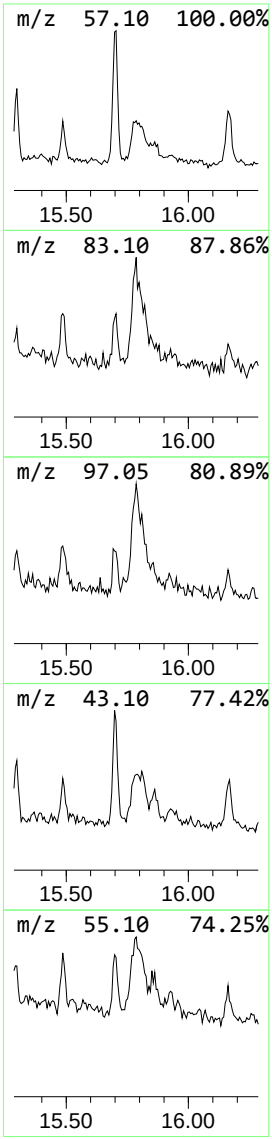
Peak Number 9 Octacosanol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.786	3.52 ng	117892	Perylene-d12	15.304

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosanol	410	C28H58O	000557-61-9	58
2	1-Tricosene	322	C23H46	018835-32-0	58
3	1-Heptacosanol	396	C27H56O	002004-39-9	58
4	n-Nonadecanol-1	284	C19H40O	001454-84-8	52
5	2-Methyl-7-nonadecene	280	C20H40	219750-68-2	42





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Operator : JU/CG
Sample : L4436-05
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 34B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101220.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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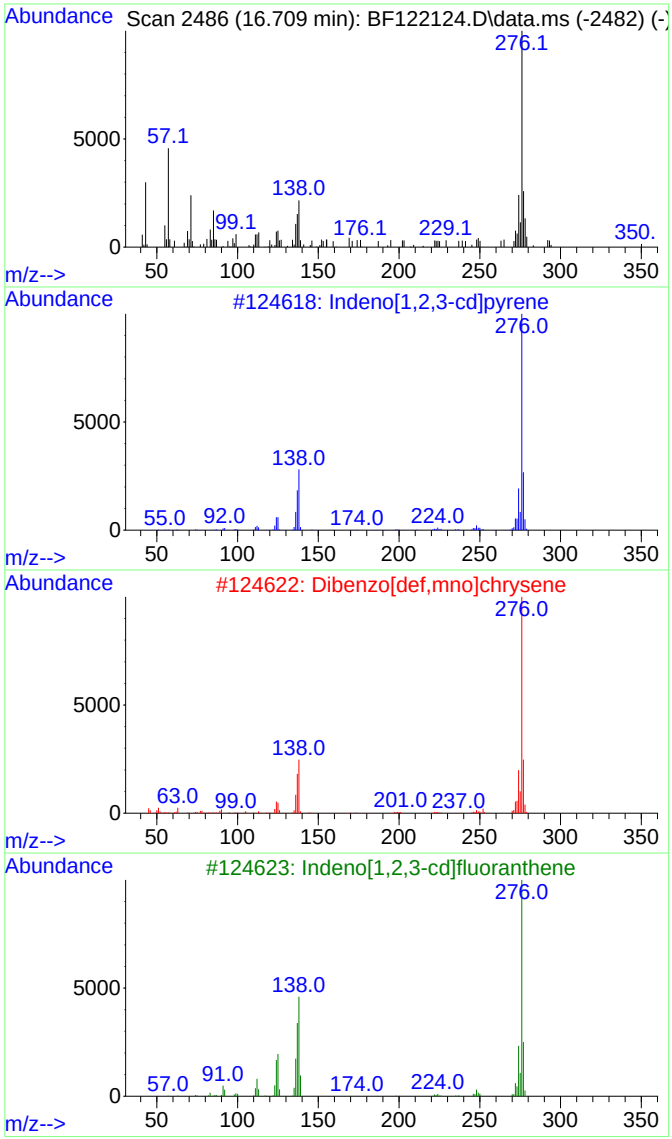
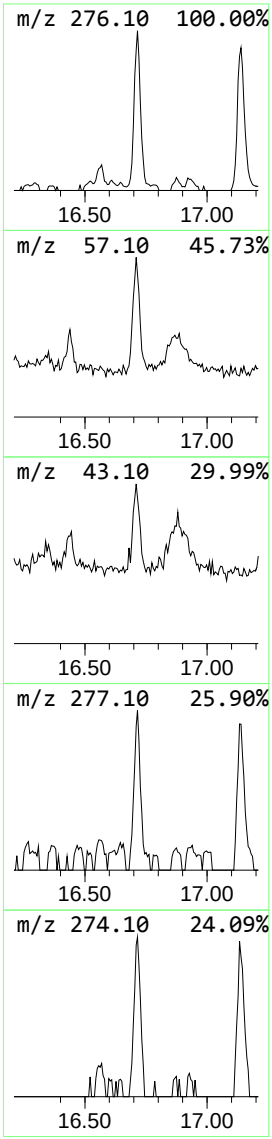
Peak Number 10 Dibenzo[def,mno]chrysene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.709	4.20 ng	140522	Perylene-d12	15.304

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Indeno[1,2,3-cd]pyrene	276	C22H12	000193-39-5	94
2	Dibenzo[def,mno]chrysene	276	C22H12	000191-26-4	93
3	Indeno[1,2,3-cd]fluoranthene	276	C22H12	000193-43-1	76
4	Benzo[ghi]perylene	276	C22H12	000191-24-2	64
5	2-Thiophenecarbaldehyde, 5-[5-(t...	276	C13H8OS3	1000217-28-5	47





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102620\
Data File : BF122124.D
Acq On : 26 Oct 2020 19:41
Operator : JU/CG
Sample : L4436-05
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 34B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101220.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
Ethanol, 2-(2-e...	6.569	2.2	ng	72099	1	6.710	655204	20.0
n-Hexadecanoic ...	11.763	2.8	ng	136615	4	11.233	967647	20.0
Heptadecyl hept...	13.716	10.0	ng	432108	5	13.874	864518	20.0
1,3-Benzenedica...	14.486	4.4	ng	190170	5	13.874	864518	20.0
Oxirane, heptad...	14.763	2.8	ng	94131	6	15.304	668921	20.0
E-7-Octadecene	15.004	5.1	ng	171444	6	15.304	668921	20.0
Perylene	15.186	3.1	ng	104326	6	15.304	668921	20.0
Nonadecane	15.698	2.5	ng	84226	6	15.304	668921	20.0
Octacosanol	15.786	3.5	ng	117892	6	15.304	668921	20.0
Dibenzo[def,mno...	16.709	4.2	ng	140522	6	15.304	668921	20.0