LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102621\
Data File : BF125948.D
Acq On : 26 Oct 2021 22:47
Operator : JU/CG
Sample : M4340-07
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TH-EES

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-BF102521.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF125948.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.163	6	13	19	rBV	2636849	3520493	83.49%	9.650%
2	5.093	508	511	515	rVB	49360	55539	1.32%	0.152%
3	5.481	572	577	580	rBV	4433592	4216541	100.00%	11.558%
4	6.487	742	748	751	rBV	4068238	4166023	98.80%	11.419%
5	6.863	809	812	816	rBV	1237960	1081885	25.66%	2.965%
6	7.428	903	908	911	rBV	2899036	2726712	64.67%	7.474%
7	8.051	1010	1014	1017	rBV	1502962	1111331	26.36%	3.046%
8	8.145	1026	1030	1034	rBV	1558405	1377804	32.68%	3.777%
9	9.222	1209	1213	1217	rBV	4109268	3858166	91.50%	10.575%
10	9.898	1325	1328	1332	rVB	1602204	1395642	33.10%	3.825%
11	10.686	1458	1462	1465	rBV	2800338	2349830	55.73%	6.441%
12	11.386	1577	1581	1583	rBV	1470504	1260486	29.89%	3.455%
13	11.410	1583	1585	1588	rVV	243711	189259	4.49%	0.519%
14	11.457	1588	1593	1596	rVB4	51407	55564	1.32%	0.152%
15	11.786	1646	1649	1654	rVB2	75239	64170	1.52%	0.176%
16	11.886	1662	1666	1668	rBV	50760	45676	1.08%	0.125%
17	11.916	1668	1671	1676	rVB	242200	218673	5.19%	0.599%
18	11.998	1681	1685	1687	rBV2	71691	79493	1.89%	0.218%
19	12.198	1717	1719	1724	rVB2	46127	45273	1.07%	0.124%
20	12.433	1756	1759	1762	rBV	59152	60774	1.44%	0.167%
21	12.598	1783	1787	1790	rBV	500907	453693	10.76%	1.244%
22	12.698	1800	1804	1807	rBV2	84832	89034	2.11%	0.244%
23	12.822	1819	1825	1828	rBV	447239	457553	10.85%	1.254%
24	12.974	1847	1851	1854	rVB	2916498	2583250	61.26%	7.081%
25	13.045	1858	1863	1866	rBV4	36953	61124	1.45%	0.168%
26	13.151	1879	1881	1884	rVB	68606	57801	1.37%	0.158%
27	13.216	1889	1892	1895	rVB2	54407	50527	1.20%	0.138%
28	13.257	1895	1899	1902	rBV2	65338	62034	1.47%	0.170%
29	13.657	1964	1967	1971	rVB	44384	52844	1.25%	0.145%
30	13.769	1983	1986	1989	rBV2	50492	63383	1.50%	0.174%
31	13.874	1999	2004	2009	rVB2	290287	307514	7.29%	0.843%
32	14.021	2024	2029	2032	rBV2	1139579	1224241	29.03%	3.356%
33	14.045	2032	2033	2036	rVB	238025	150075	3.56%	0.411%
34	14.204	2058	2060	2063	rVB2	48343	46576	1.10%	0.128%
35	14.410	2092	2095	2098	rVB	48963	44589	1.06%	0.122%
36	14.445	2098	2101	2104	rVB	54228	50131	1.19%	0.137%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102621\
Data File : BF125948.D
Acq On : 26 Oct 2021 22:47
Operator : JU/CG
Sample : M4340-07
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TH-EES

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-BF102521.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	14.510	2108	2112	2118	rBV2	284279	330571	7.84%	0.906%
38	14.898	2175	2178	2183	rVB2	85087	96661	2.29%	0.265%
39	15.063	2201	2206	2209	rBV	257210	381393	9.05%	1.045%
40	15.168	2221	2224	2230	rVB2	71781	137271	3.26%	0.376%
41	15.363	2254	2257	2263	rVB	151317	187771	4.45%	0.515%
42	15.427	2264	2268	2274	rVB	211000	244720	5.80%	0.671%
43	15.492	2274	2279	2283	rBV2	863417	1068983	25.35%	2.930%
44	16.039	2369	2372	2380	rVB7	49521	87689	2.08%	0.240%
45	16.951	2521	2527	2536	rVB3	91306	199471	4.73%	0.547%
46	17.386	2596	2601	2608	rVB	65127	114899	2.72%	0.315%

Sum of corrected areas: 36483132

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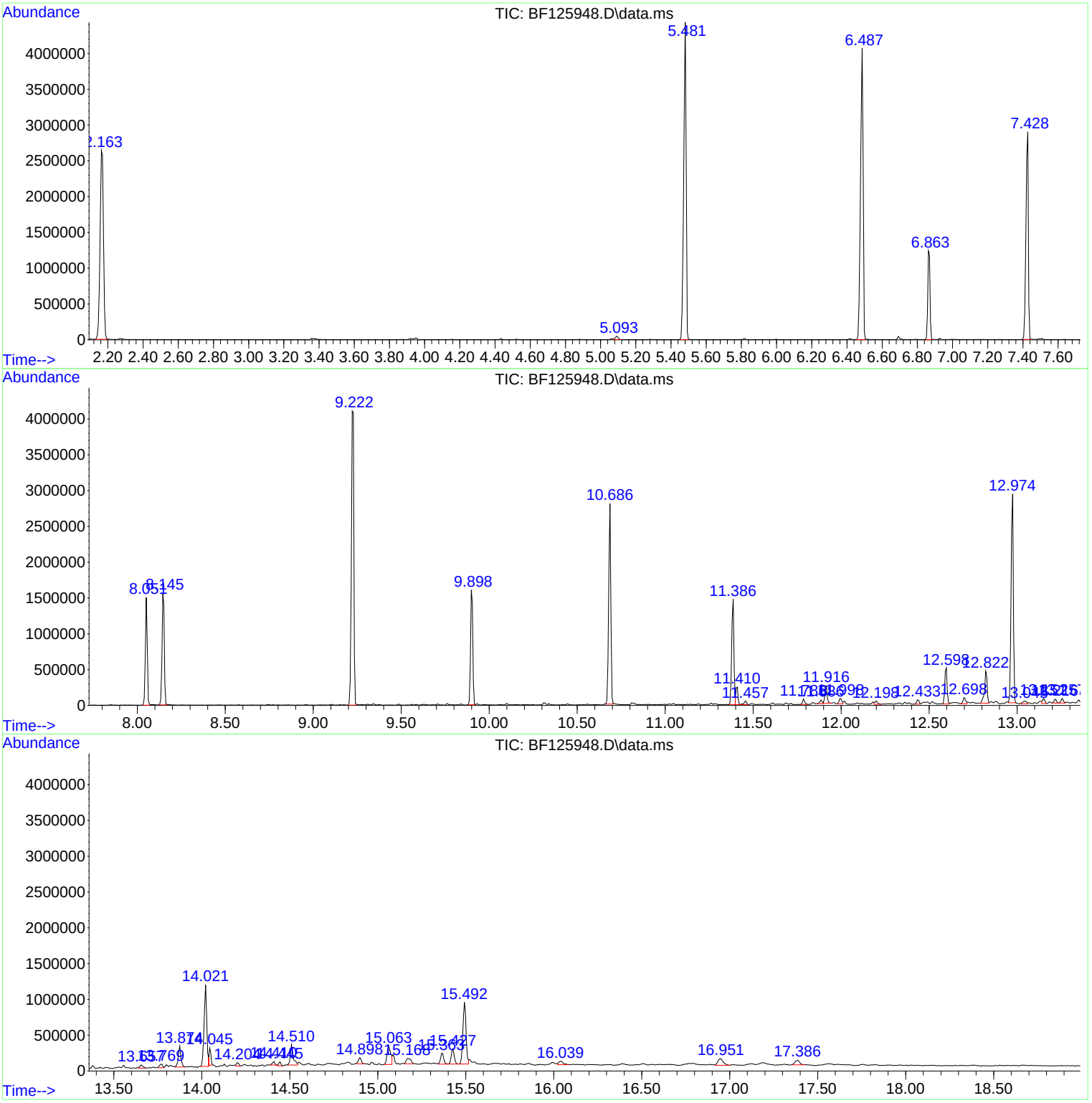
Sample : M4340-07
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TH-EES

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF102521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102621\
Data File : BF125948.D
Acq On : 26 Oct 2021 22:47
Operator : JU/CG
Sample : M4340-07
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TH-EES

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF102521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

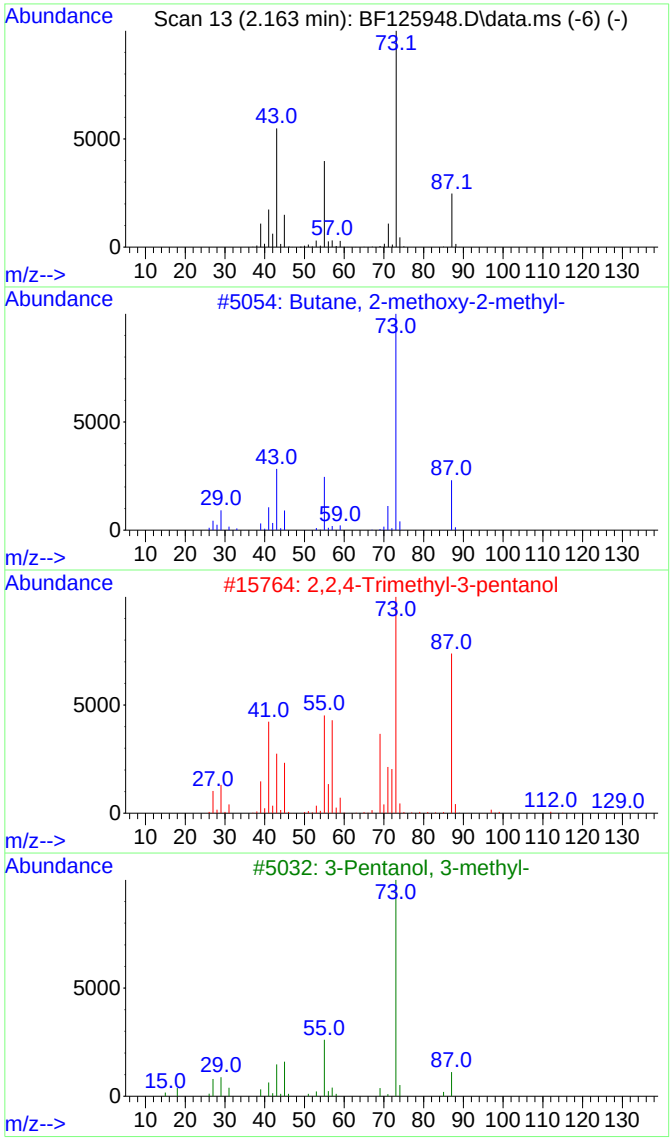
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

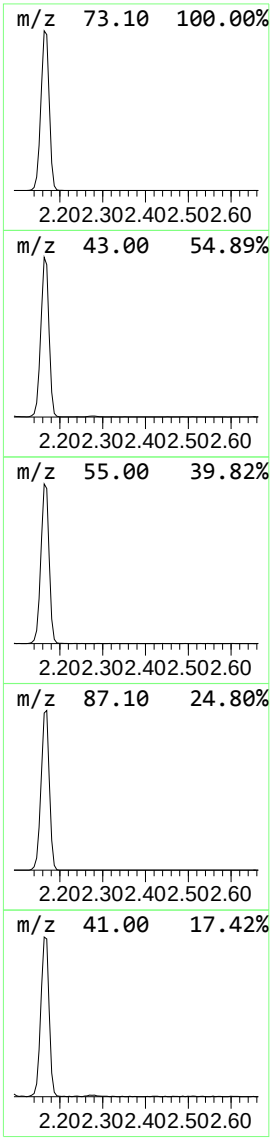
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.163	65.08 ng	3520490	1,4-Dichlorobenzene-d4	6.869

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3	3-Pentanol, 3-methyl-	102	C6H14O	000077-74-7	32
4	Silane, tetramethyl-	88	C4H12Si	000075-76-3	25
5	3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	17





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102621\
Data File : BF125948.D
Acq On : 26 Oct 2021 22:47
Operator : JU/CG
Sample : M4340-07
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TH-EES

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF102521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

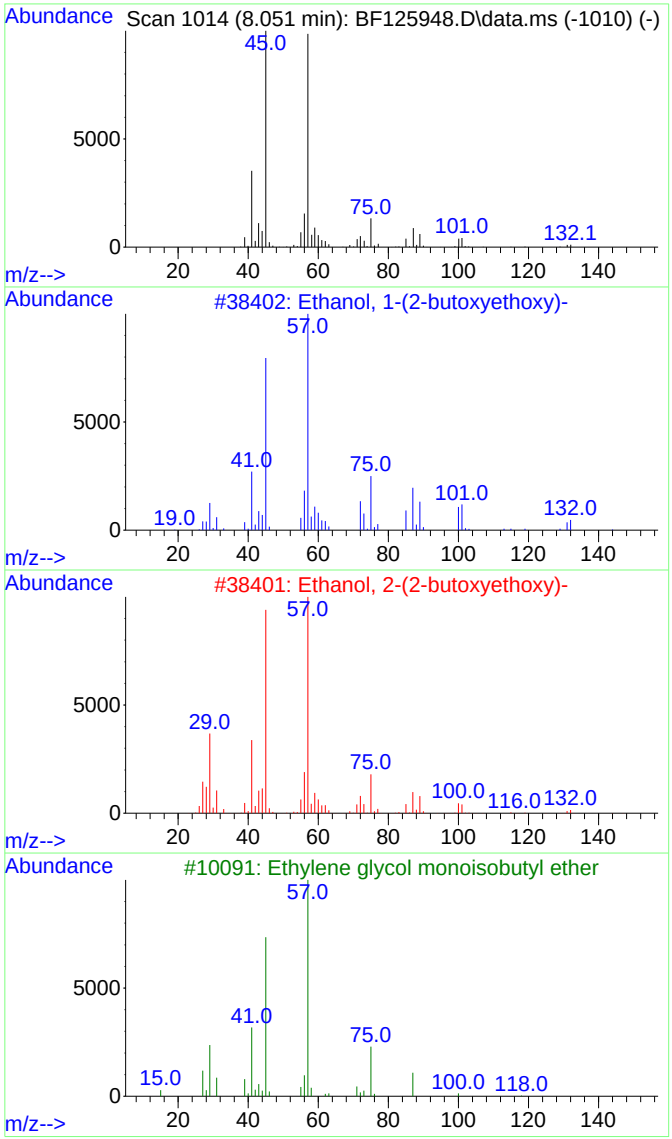
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

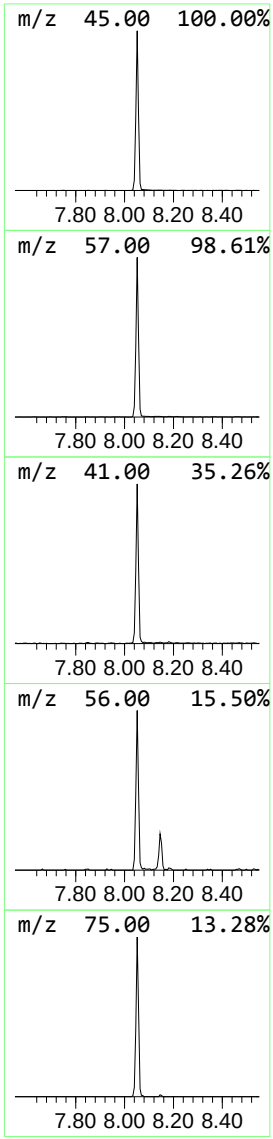
****

Peak Number 2 Ethanol, 1-(2-butoxyethoxy)- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.051	16.13 ng	1111330	Naphthalene-d8	8.145

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	50
2	Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	50
3	Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	45
4	Butane, 1-methoxy-	88	C5H12O	000628-28-4	43
5	2-Hexanol	102	C6H14O	000626-93-7	43





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102621\
Data File : BF125948.D
Acq On : 26 Oct 2021 22:47
Operator : JU/CG
Sample : M4340-07
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TH-EES

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF102521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

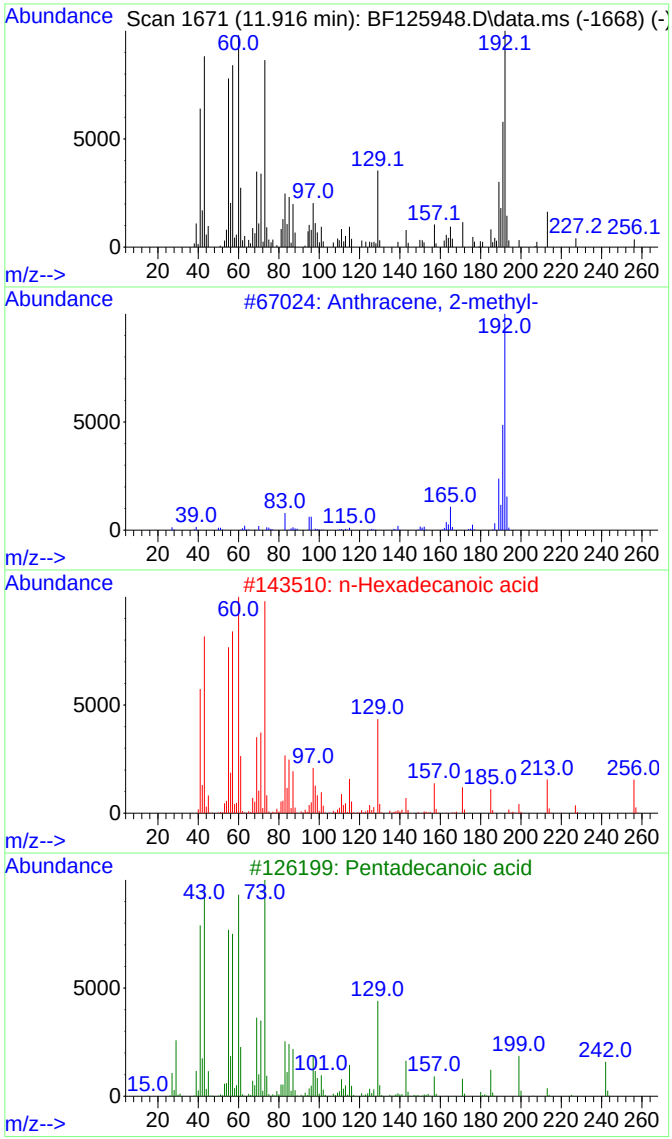
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

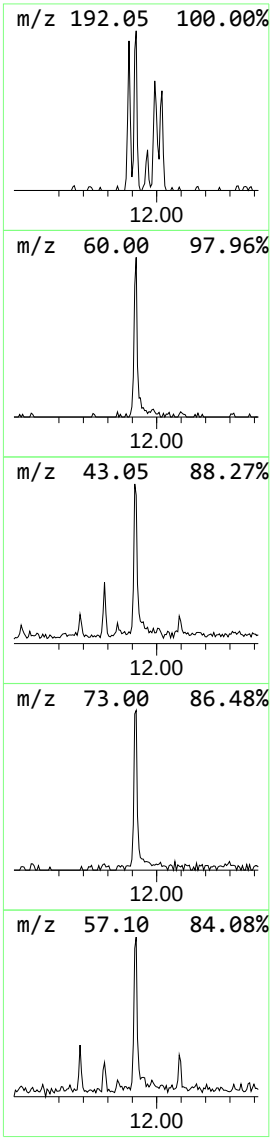
****

Peak Number 3 Anthracene, 2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.916	3.47 ng	218673	Phenanthrene-d10	11.386

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Anthracene, 2-methyl-	192	C15H12	000613-12-7	70
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	70
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	55
4	Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	51
5	Phenanthrene, 3-methyl-	192	C15H12	000832-71-3	38





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102621\
Data File : BF125948.D
Acq On : 26 Oct 2021 22:47
Operator : JU/CG
Sample : M4340-07
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TH-EES

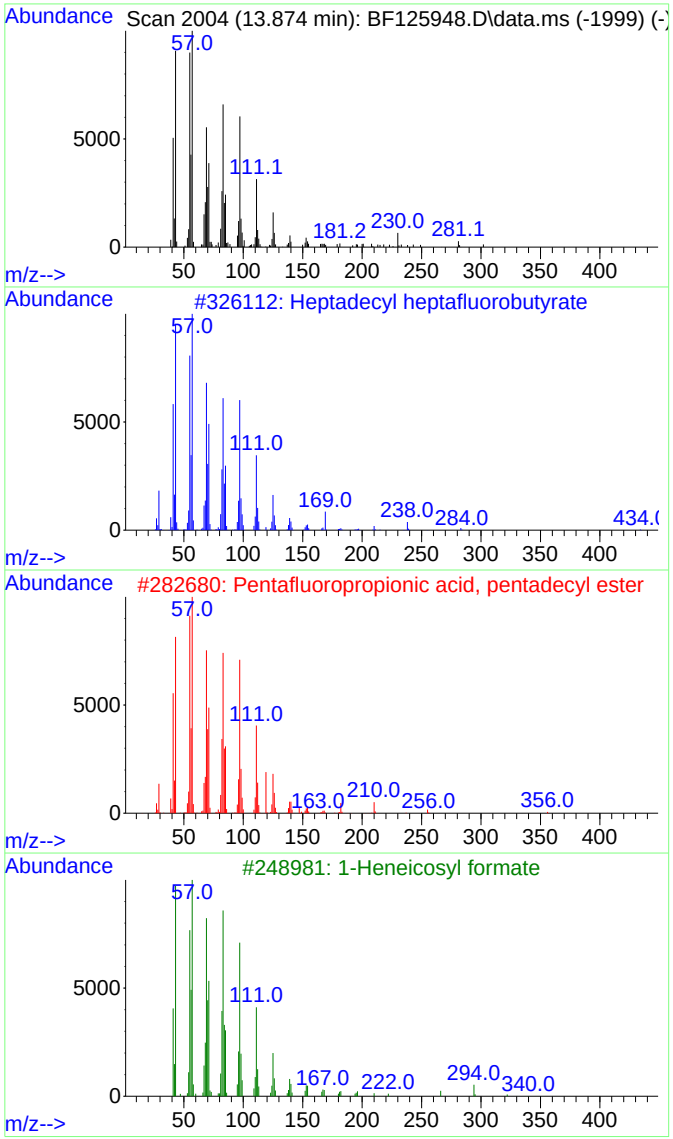
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF102521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

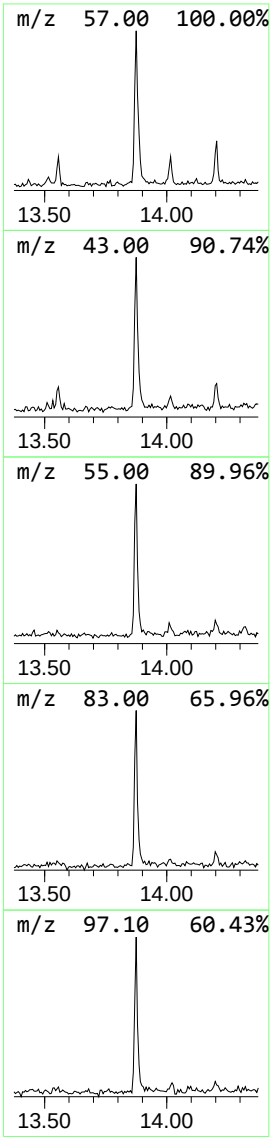
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Heptadecyl heptafluorobutyrate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.874	5.02 ng	307514	Chrysene-d12	14.021

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	93
2	Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	91
3	1-Heneicosyl formate	340	C22H44O2	077899-03-7	91
4	Pentafluoropropionic acid, hepta...	402	C20H35F5O2	959218-78-1	90
5	Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	90





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102621\
Data File : BF125948.D
Acq On : 26 Oct 2021 22:47
Operator : JU/CG
Sample : M4340-07
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TH-EES

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF102521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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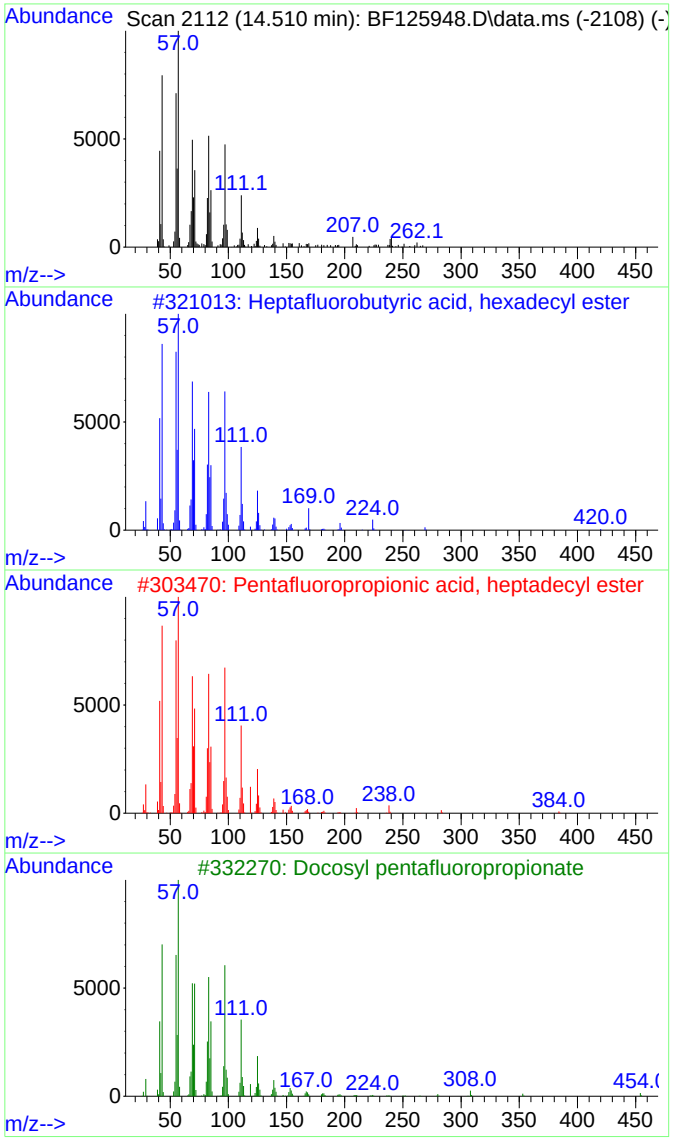
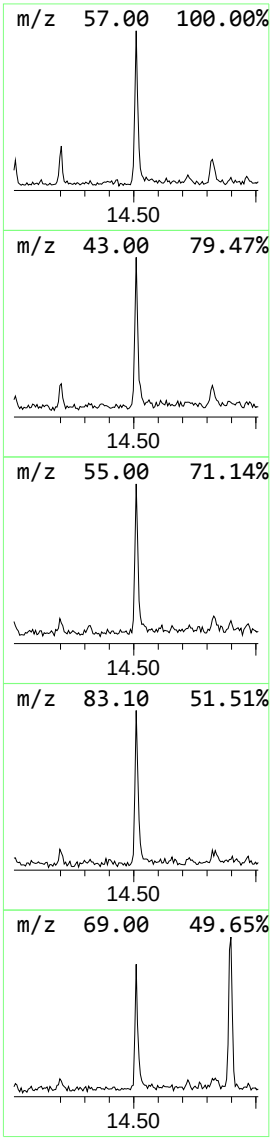
Peak Number 5 Heptafluorobutyric acid, he... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.510	5.40 ng	330571	Chrysene-d12	14.021

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptafluorobutyric acid, hexadec...	438	C20H33F7O2	006385-15-5	94
2	Pentafluoropropionic acid, hepta...	402	C20H35F5O2	959218-78-1	91
3	Docosyl pentafluoropropionate	472	C25H45F5O2	1000351-80-9	91
4	Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	91
5	Pentafluoropropionic acid, octad...	416	C21H37F5O2	959261-25-7	91





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Data File : BF125948.D
Acq On : 26 Oct 2021 22:47
Operator : JU/CG
Sample : M4340-07
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TH-EES

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF102521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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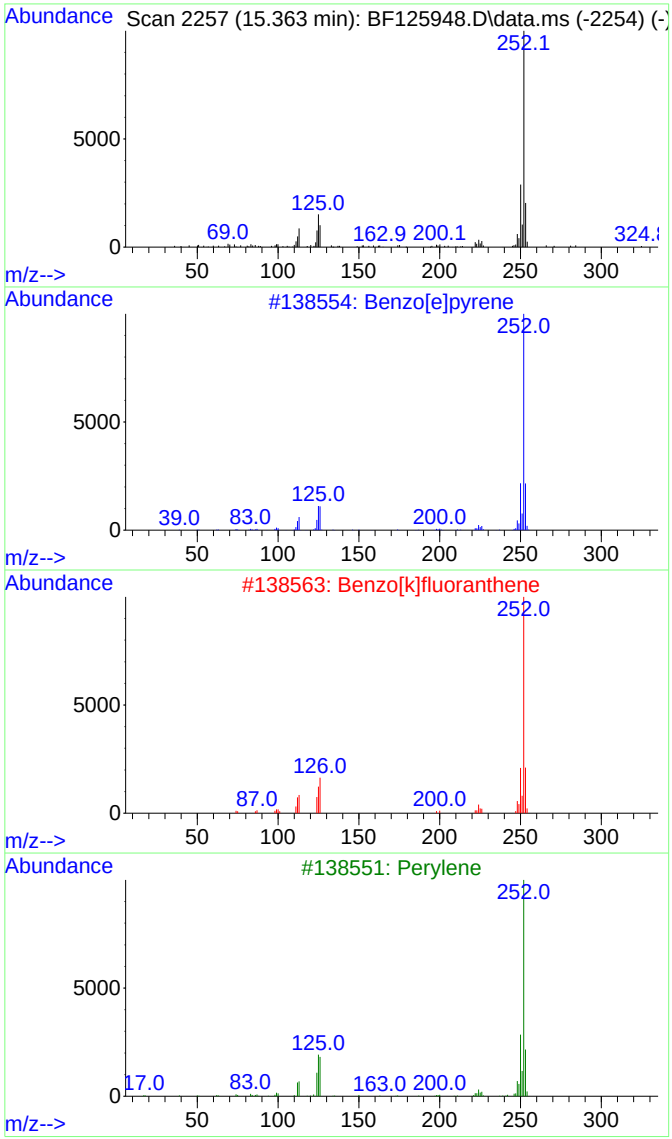
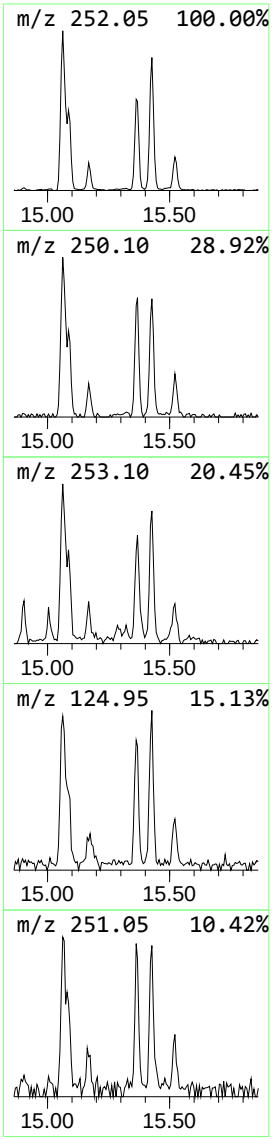
Peak Number 7 Benzo[e]pyrene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.363	3.51 ng	187771	Perylene-d12	15.492

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[e]pyrene	252	C20H12	000192-97-2	98
2	Benzo[k]fluoranthene	252	C20H12	000207-08-9	96
3	Perylene	252	C20H12	000198-55-0	94
4	Benzo[b]fluoranthene	252	C20H12	000205-99-2	93
5	Benzo[a]pyrene	252	C20H12	000050-32-8	93





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102621\
Data File : BF125948.D
Acq On : 26 Oct 2021 22:47
Operator : JU/CG
Sample : M4340-07
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TH-EES

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF102521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Butane, 2-metho...	2.163	65.1	ng	3520490	1	6.869	1081890	20.0
Ethanol, 1-(2-b...	8.051	16.1	ng	1111330	2	8.145	1377800	20.0
Anthracene, 2-m...	11.916	3.5	ng	218673	4	11.386	1260490	20.0
Heptadecyl hept...	13.874	5.0	ng	307514	5	14.021	1224240	20.0
Heptafluorobuty...	14.510	5.4	ng	330571	5	14.021	1224240	20.0
Benzo[e]pyrene	15.363	3.5	ng	187771	6	15.492	1068980	20.0