LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF101821\
Data File : BF125880.D
Acq On : 18 Oct 2021 16:44
Operator : JU/CG
Sample : M4252-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TEST-BA-(1)

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-BF100721.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF125880.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.439	565	570	573	rBV	3304058	3068741	84.44%	11.137%
2	6.451	736	742	745	rBV	3022906	3048193	83.87%	11.062%
3	6.822	801	805	808	rBV	1213721	904278	24.88%	3.282%
4	7.381	895	900	903	rBV	2227787	1971259	54.24%	7.154%
5	8.004	1002	1006	1019	rBV	256164	218393	6.01%	0.793%
6	8.104	1019	1023	1026	rBV	1450460	1249808	34.39%	4.536%
7	9.175	1201	1205	1209	rBV	3967661	3634312	100.00%	13.189%
8	9.716	1294	1297	1303	rBV	46474	40861	1.12%	0.148%
9	9.857	1317	1321	1324	rBV	1483808	1354144	37.26%	4.914%
10	10.639	1450	1454	1457	rBV	2322764	1962306	53.99%	7.121%
11	11.333	1569	1572	1575	rBV	1270921	1138622	31.33%	4.132%
12	11.357	1575	1576	1580	rVV	206701	140089	3.85%	0.508%
13	11.410	1580	1585	1588	rVB2	49372	50088	1.38%	0.182%
14	11.839	1653	1658	1659	rBV	49679	44164	1.22%	0.160%
15	11.863	1659	1662	1666	rVB	135081	117934	3.25%	0.428%
16	11.945	1673	1676	1679	rBV	68602	75437	2.08%	0.274%
17	12.386	1747	1751	1754	rBV	51972	47254	1.30%	0.171%
18	12.468	1762	1765	1770	rVB	39008	39432	1.08%	0.143%
19	12.545	1774	1778	1782	rVB	567506	461286	12.69%	1.674%
20	12.639	1792	1794	1797	rBV	46593	43143	1.19%	0.157%
21	12.774	1811	1817	1820	rBV	524188	487328	13.41%	1.769%
22	12.921	1838	1842	1845	rVV	2823772	2469770	67.96%	8.963%
23	12.992	1848	1854	1857	rBV2	44837	69569	1.91%	0.252%
24	13.104	1870	1873	1876	rVB2	78753	72234	1.99%	0.262%
25	13.168	1876	1884	1887	rBV2	49444	69747	1.92%	0.253%
26	13.204	1887	1890	1894	rVV2	66104	66938	1.84%	0.243%
27	13.327	1909	1911	1916	rBV2	43668	41969	1.15%	0.152%
28	13.504	1934	1941	1943	rBV6	25633	48186	1.33%	0.175%
29	13.604	1951	1958	1963	rBV	58343	76105	2.09%	0.276%
30	13.721	1973	1978	1981	rBV2	55454	84810	2.33%	0.308%
31	13.815	1990	1994	2004	rVB4	142581	191945	5.28%	0.697%
32	13.968	2015	2020	2023	rBV2	1238559	1350262	37.15%	4.900%
33	13.992	2023	2024	2031	rVB	299372	250459	6.89%	0.909%
34	14.192	2054	2058	2061	rBV2	26008	38009	1.05%	0.138%
35	14.357	2082	2086	2089	rBV2	73161	69473	1.91%	0.252%
36	14.386	2089	2091	2094	rVB2	51815	48402	1.33%	0.176%

LSC Area Percent Report

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Misc :
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Instrument : BNA_F
ClientSampleId : TEST-BA-(1)

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-BF100721.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	14.451	2099	2102	2104	rBV2	44209	46882	1.29%	0.170%
38	14.551	2115	2119	2123	rVB4	26694	43883	1.21%	0.159%
39	14.739	2148	2151	2154	rBV5	28512	38382	1.06%	0.139%
40	14.821	2162	2165	2168	rBV3	57190	62077	1.71%	0.225%
41	14.998	2190	2195	2198	rBV	294377	447844	12.32%	1.625%
42	15.104	2210	2213	2217	rVB	62499	64406	1.77%	0.234%
43	15.292	2241	2245	2251	rVB	167895	218607	6.02%	0.793%
44	15.356	2251	2256	2261	rBV	241086	287701	7.92%	1.044%
45	15.415	2261	2266	2270	rVV	744505	925891	25.48%	3.360%
46	15.445	2270	2271	2278	rVB3	76035	97647	2.69%	0.354%
47	16.851	2504	2510	2518	rVB2	78120	160823	4.43%	0.584%
48	17.274	2577	2582	2592	rBV	63365	116330	3.20%	0.422%

Sum of corrected areas: 27555423

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ClientSampleId :
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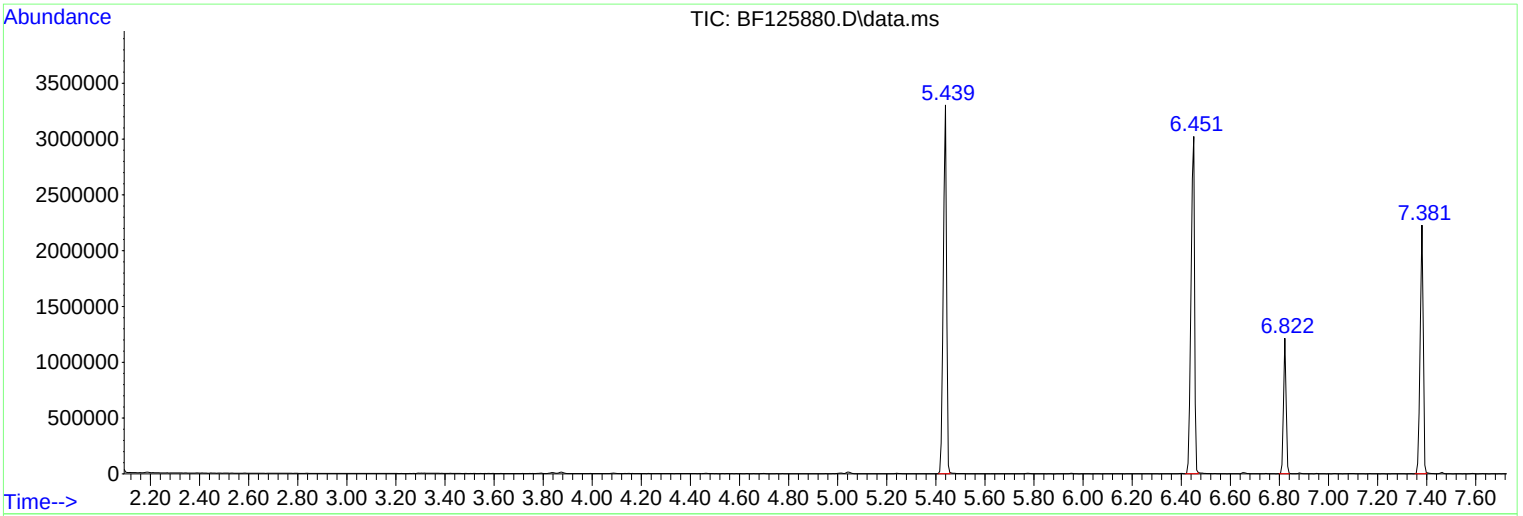
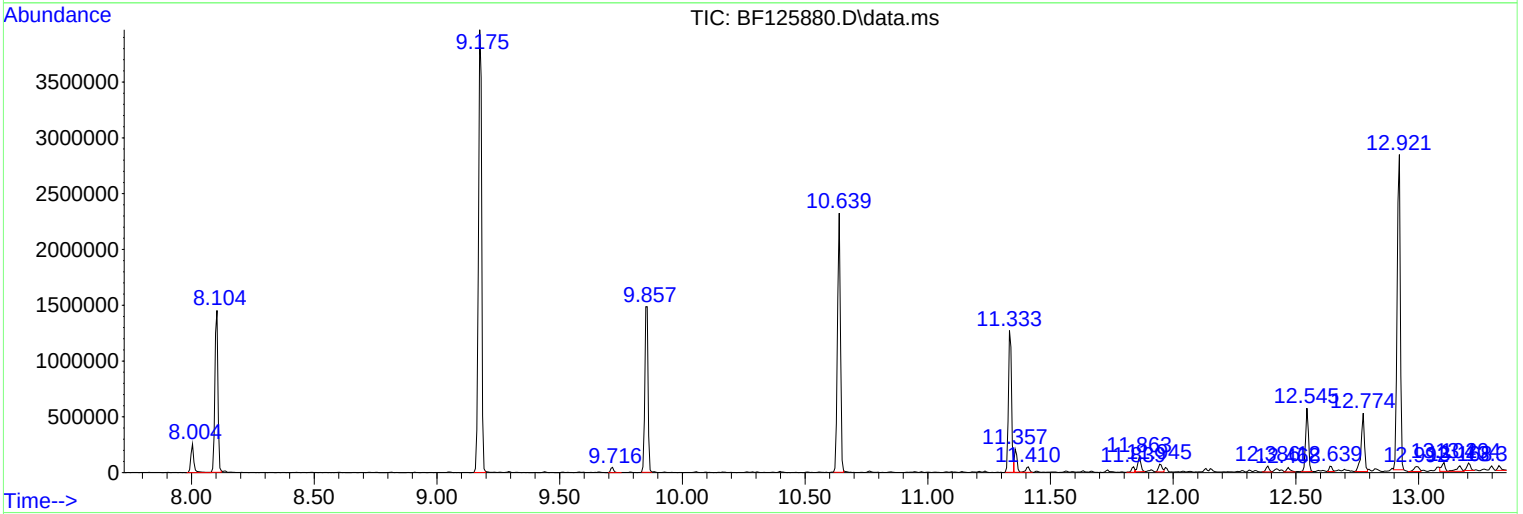
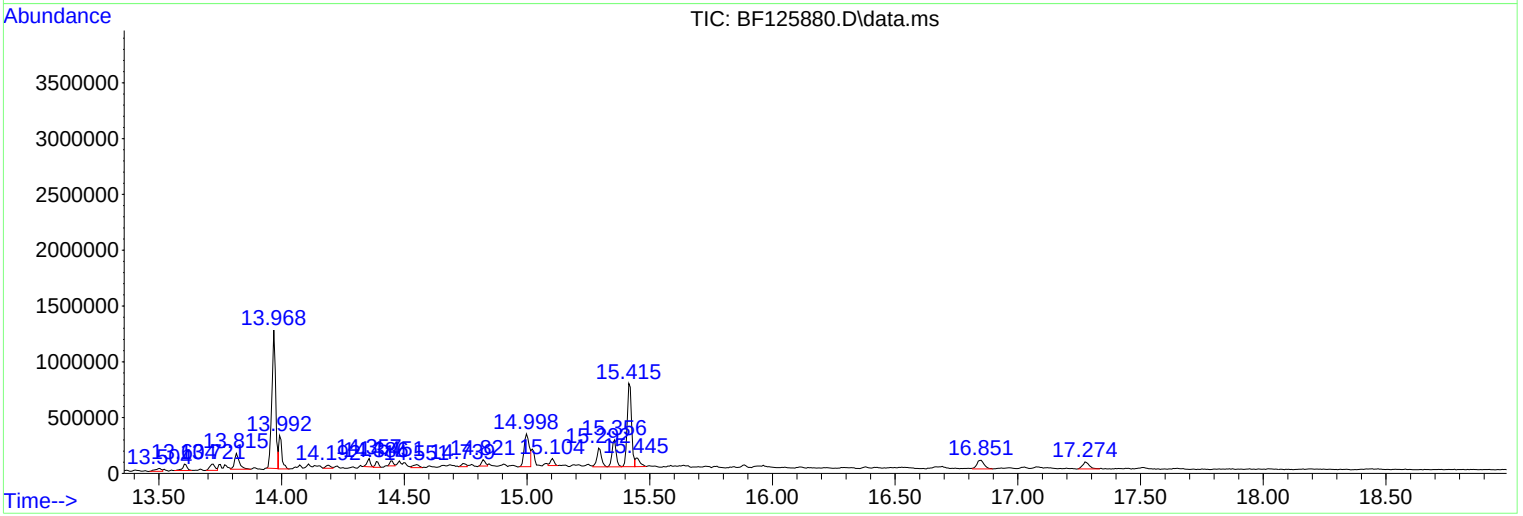
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF100721.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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







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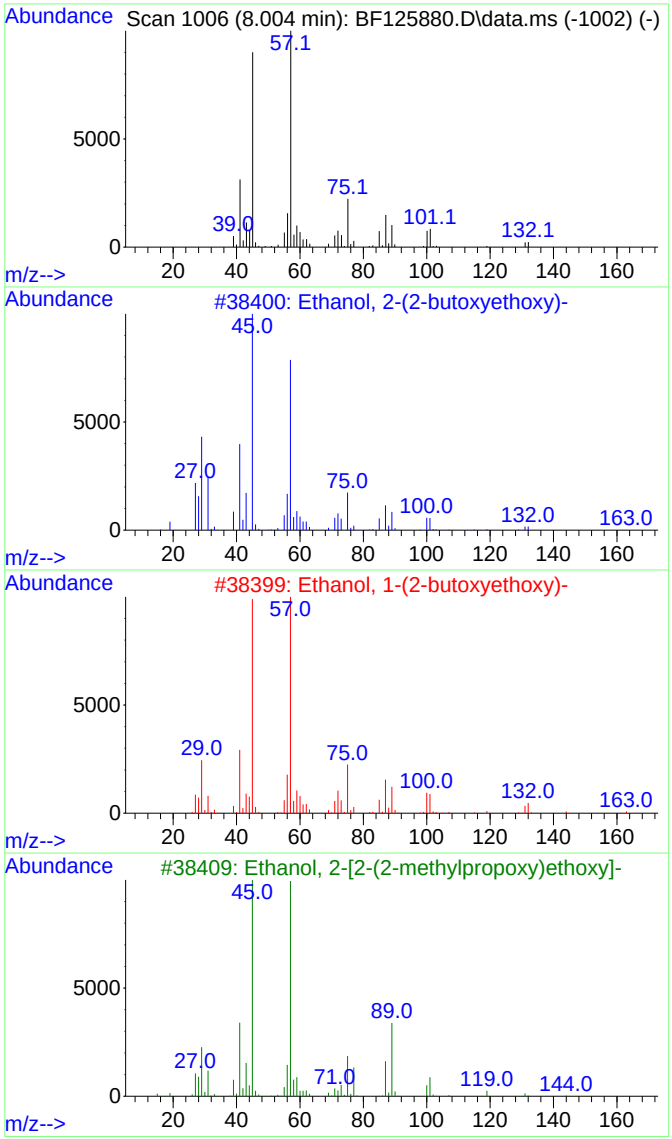
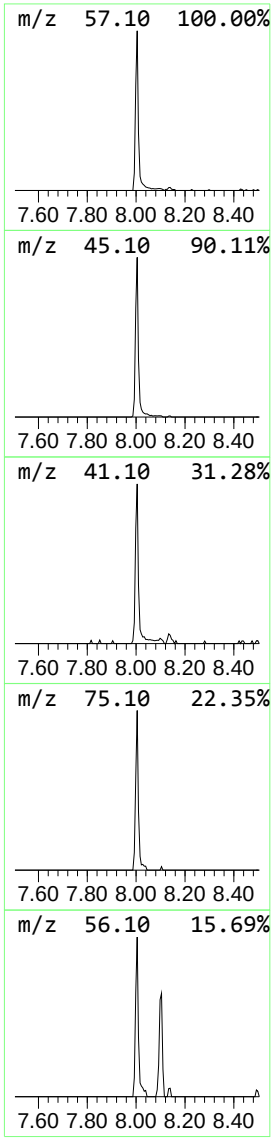
****
Peak Number 1 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.004	3.49 ng	218393	Naphthalene-d8	8.104

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
2	Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	83
3	Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	72
4	Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	64
5	Ethanol, 2-[2-(2-butoxyethoxy)et...	206	C10H22O4	000143-22-6	59





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Instrument :
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ClientSampleId :
TEST-BA-(1)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF100721.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

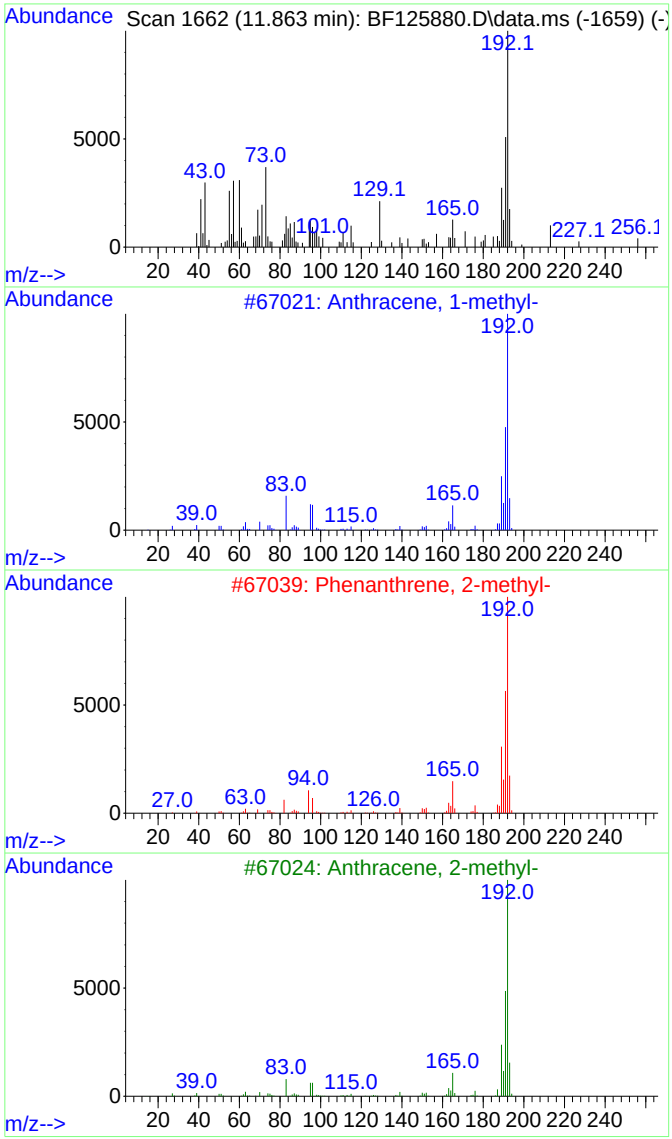
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

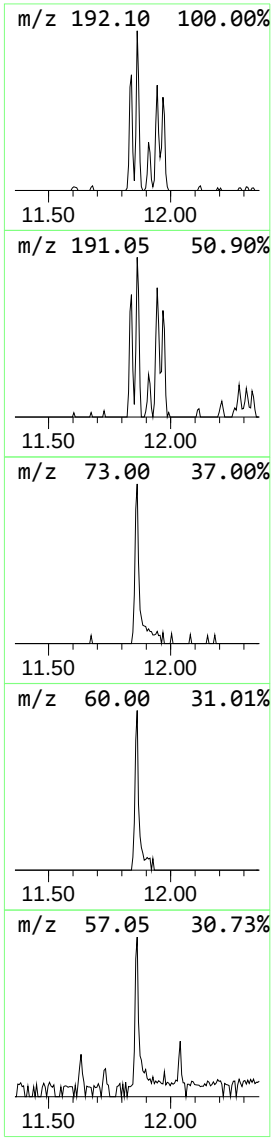
****

Peak Number 2 Anthracene, 1-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.863	2.07 ng	117934	Phenanthrene-d10	11.333

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Anthracene, 1-methyl-	192	C15H12	000610-48-0	95
2	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	91
3	Anthracene, 2-methyl-	192	C15H12	000613-12-7	90
4	Naphtho[2,3-b]norbornadiene	192	C15H12	107426-38-0	90
5	Anthracene, 9-methyl-	192	C15H12	000779-02-2	78





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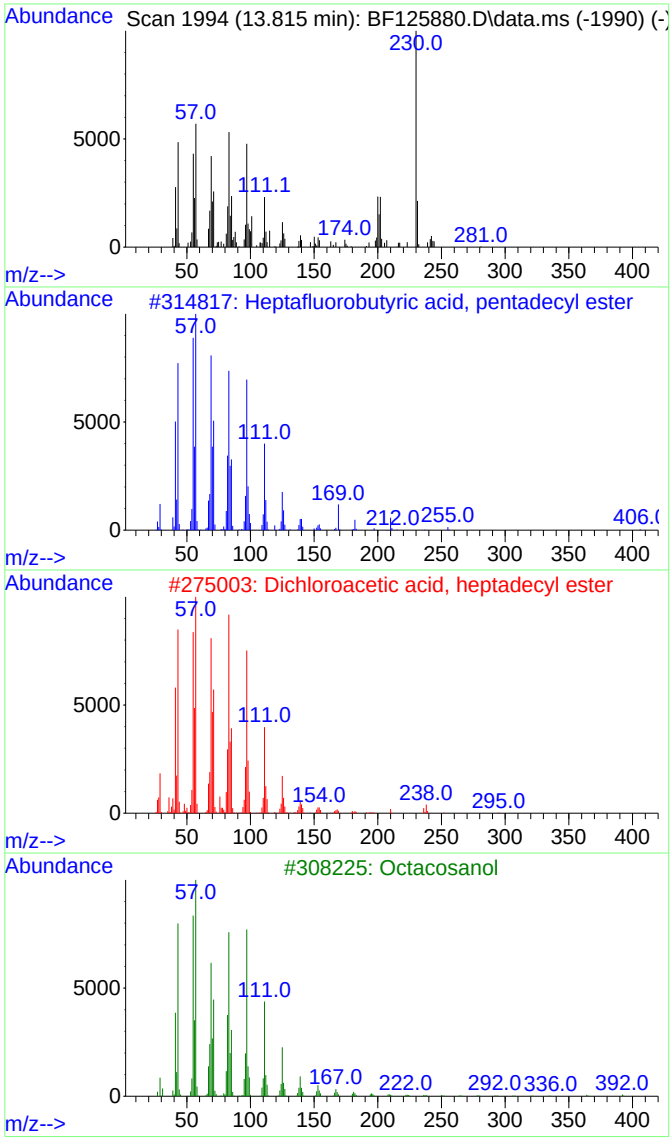
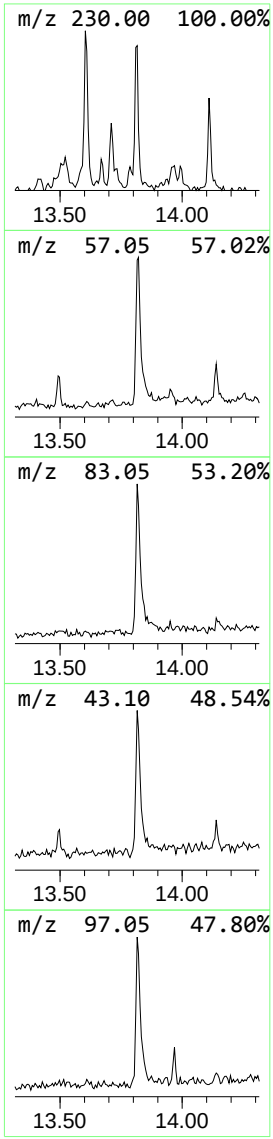
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Heptafluorobutyric acid, pe... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.815	2.84 ng	191945	Chrysene-d12	13.968

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	83
2	Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	83
3	Octacosanol	410	C28H58O	000557-61-9	81
4	Pentafluoropropionic acid, hepta...	402	C20H35F5O2	959218-78-1	80
5	1-Hexacosene	364	C26H52	018835-33-1	80





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Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF100721.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

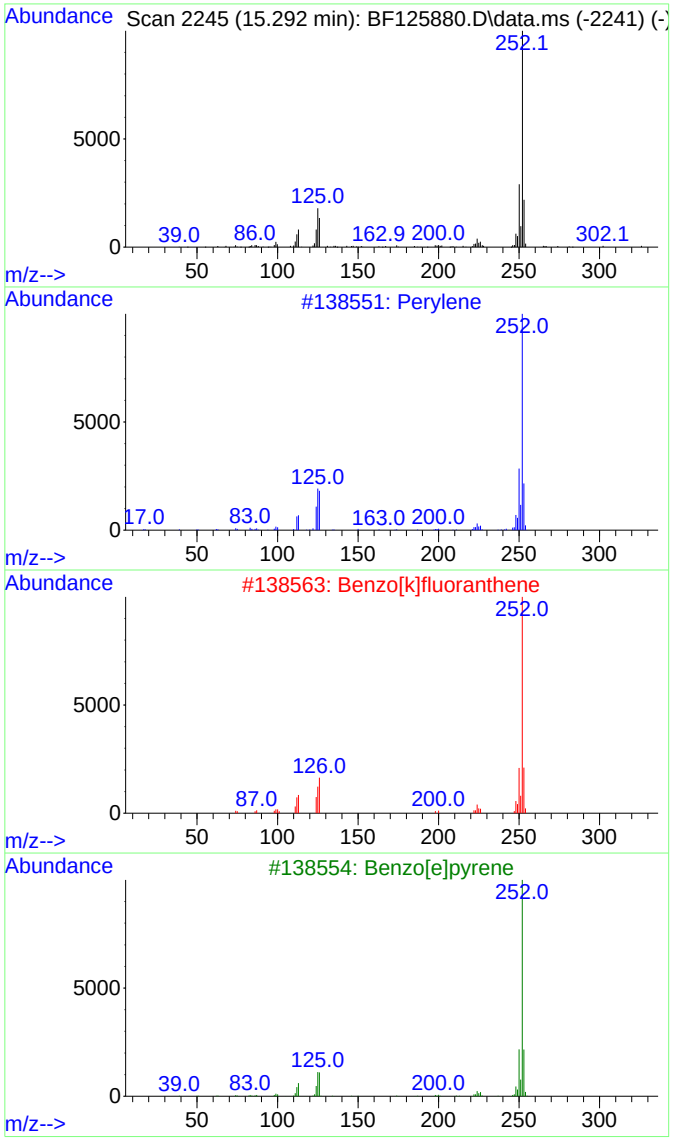
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

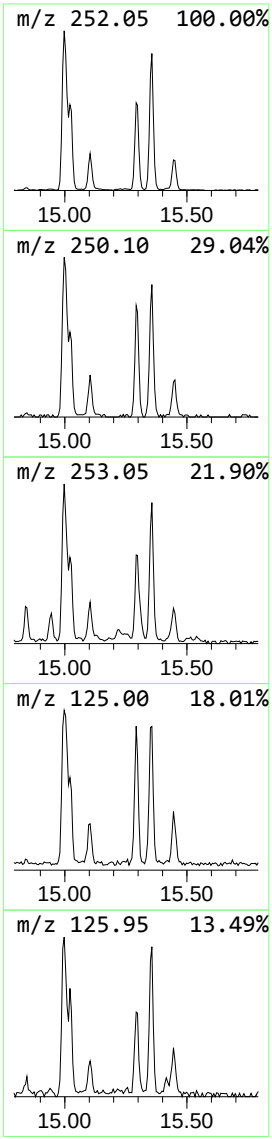
****

Peak Number 4 Perylene Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.292	4.72 ng	218607	Perylene-d12	15.415

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Perylene	252	C20H12	000198-55-0	99
2	Benzo[k]fluoranthene	252	C20H12	000207-08-9	98
3	Benzo[e]pyrene	252	C20H12	000192-97-2	97
4	Benzo[j]fluoranthene	252	C20H12	000205-82-3	96
5	Benzo[a]pyrene	252	C20H12	000050-32-8	93





Tentatively Identified Compound (LSC) summary

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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
Ethanol, 2-(2-b...	8.004	3.5	ng	218393	2	8.104	1249810	20.0
Anthracene, 1-m...	11.863	2.1	ng	117934	4	11.333	1138620	20.0
Heptafluorobuty...	13.815	2.8	ng	191945	5	13.968	1350260	20.0
Perylene	15.292	4.7	ng	218607	6	15.415	925891	20.0