LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF041621\
Data File : BF123592.D
Acq On : 16 Apr 2021 14:53
Operator : JU/CG
Sample : M2048-18
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-06-8.5-9.0

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-BF041521.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF123592.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.116	3	5	16	rVB	2088994	2084328	37.23%	4.725%
2	5.481	572	577	580	rBV	5903306	5346153	95.49%	12.118%
3	6.492	744	749	752	rBV	5587422	5598736	100.00%	12.691%
4	6.869	809	813	816	rBV	1424387	1264538	22.59%	2.866%
5	7.428	903	908	911	rBV	4128446	3618877	64.64%	8.203%
6	8.151	1027	1031	1034	rBV	2150231	1631899	29.15%	3.699%
7	9.233	1210	1215	1218	rBV	6563028	5303758	94.73%	12.022%
8	9.622	1278	1281	1285	rBV	237231	177891	3.18%	0.403%
9	9.910	1326	1330	1334	rBV	2015837	1767848	31.58%	4.007%
10	10.704	1460	1465	1468	rBV	4303150	4153721	74.19%	9.415%
11	11.398	1580	1583	1587	rBV	2149961	1906405	34.05%	4.321%
12	11.933	1669	1674	1681	rBV	380364	429134	7.66%	0.973%
13	12.992	1850	1854	1857	rBV	5682055	5191371	92.72%	11.768%
14	13.063	1862	1866	1869	rBV	415092	344284	6.15%	0.780%
15	13.227	1891	1894	1904	rVB	77852	80856	1.44%	0.183%
16	13.568	1950	1952	1955	rBV	88991	77940	1.39%	0.177%
17	13.686	1968	1972	1977	rVB3	55767	65995	1.18%	0.150%
18	13.904	2002	2009	2023	rBV2	515906	1123604	20.07%	2.547%
19	14.045	2029	2033	2039	rVB	1602261	1623187	28.99%	3.679%
20	14.221	2059	2063	2066	rBV	119801	117916	2.11%	0.267%
21	14.527	2111	2115	2117	rBV	139810	121669	2.17%	0.276%
22	14.839	2164	2168	2173	rBV	92576	96469	1.72%	0.219%
23	15.186	2223	2227	2232	rVB	74505	80752	1.44%	0.183%
24	15.533	2280	2286	2291	rBV2	991438	1291037	23.06%	2.926%
25	15.574	2291	2293	2301	rVB2	73613	101170	1.81%	0.229%
26	17.727	2654	2659	2666	rVB7	100468	216017	3.86%	0.490%
27	18.021	2699	2709	2726	rBV7	58954	300284	5.36%	0.681%

Sum of corrected areas: 44115839

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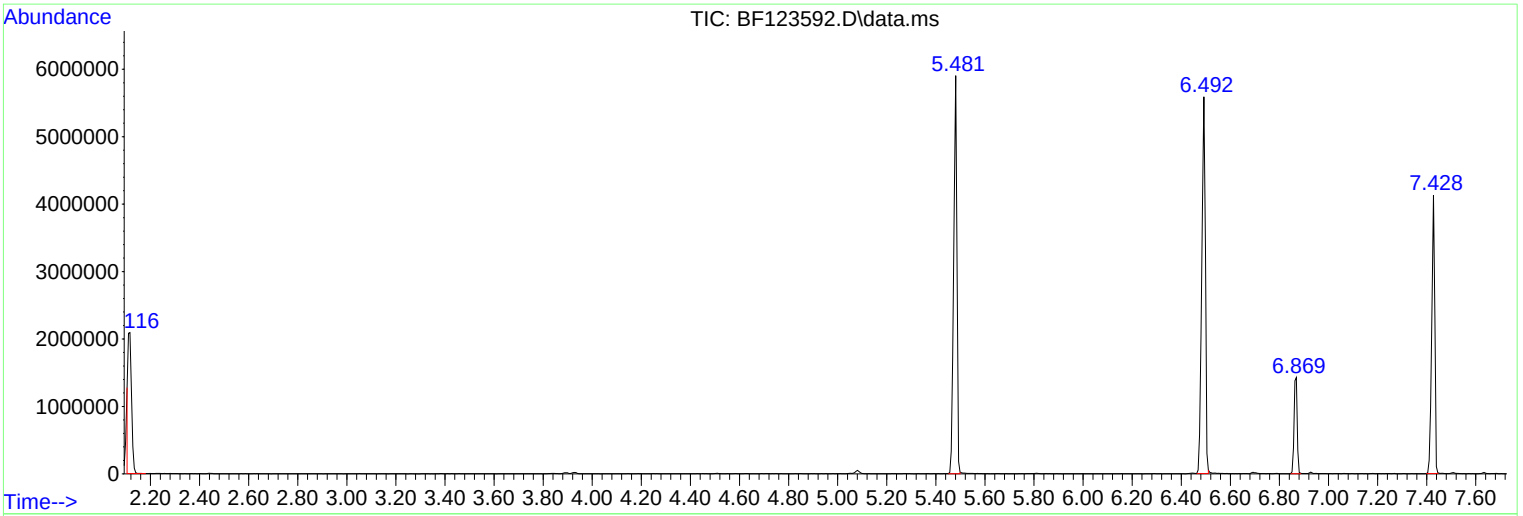
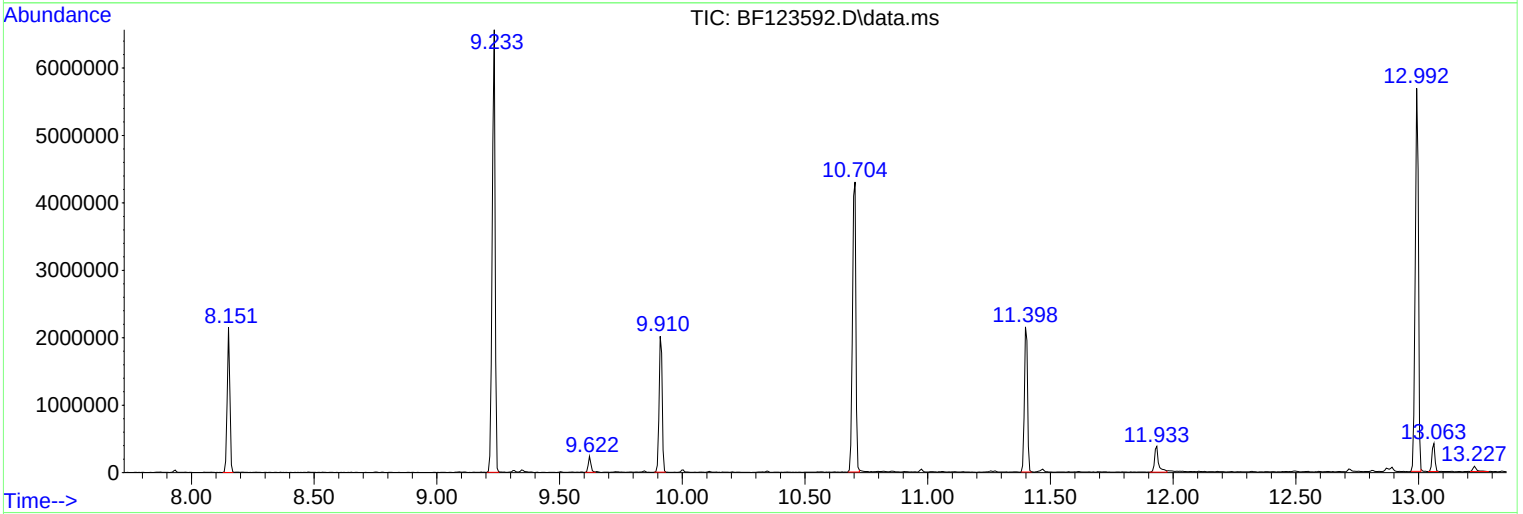
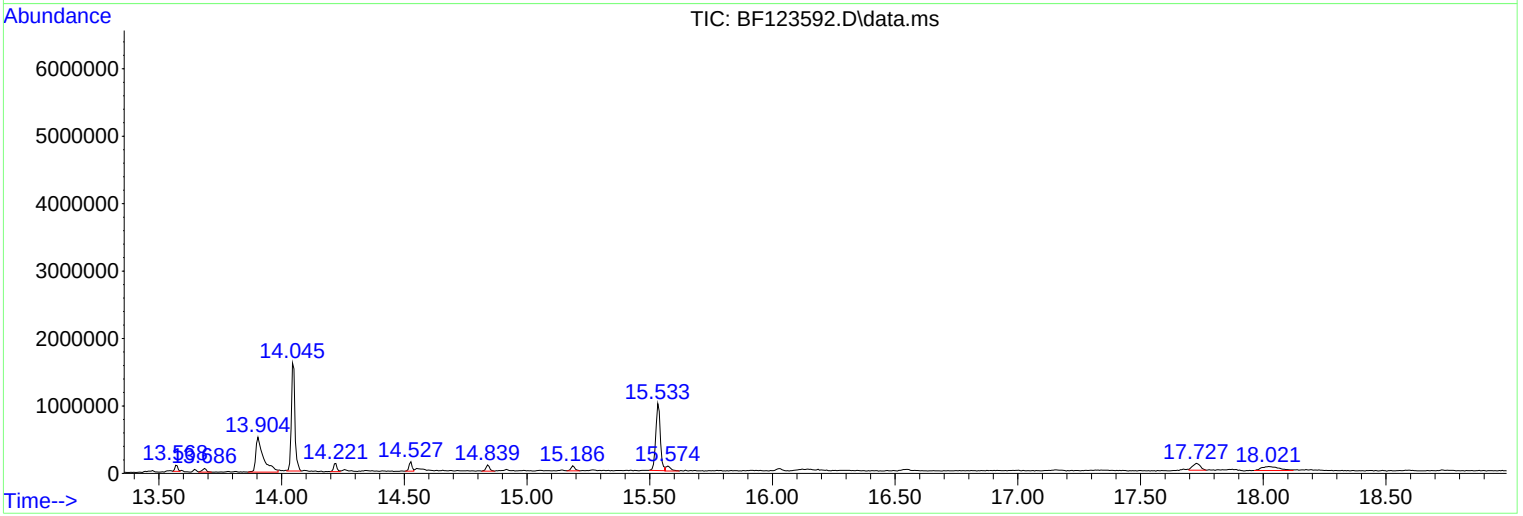
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF041521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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







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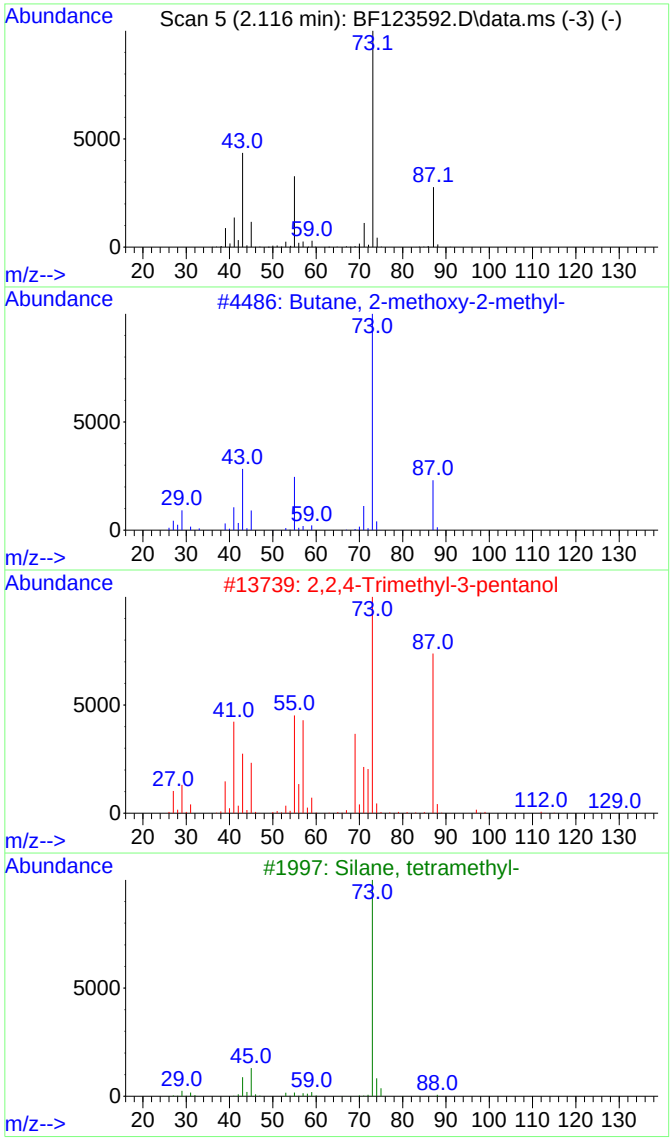
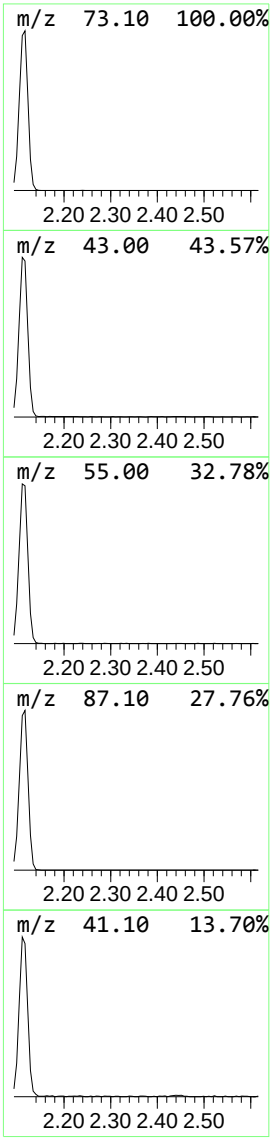
****
Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.116	32.97 ng	2084330	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	Silane, tetramethyl-	88	C4H12Si	000075-76-3	38
4	N-Ethylformamide	73	C3H7NO	000627-45-2	9
5	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	9





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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF041521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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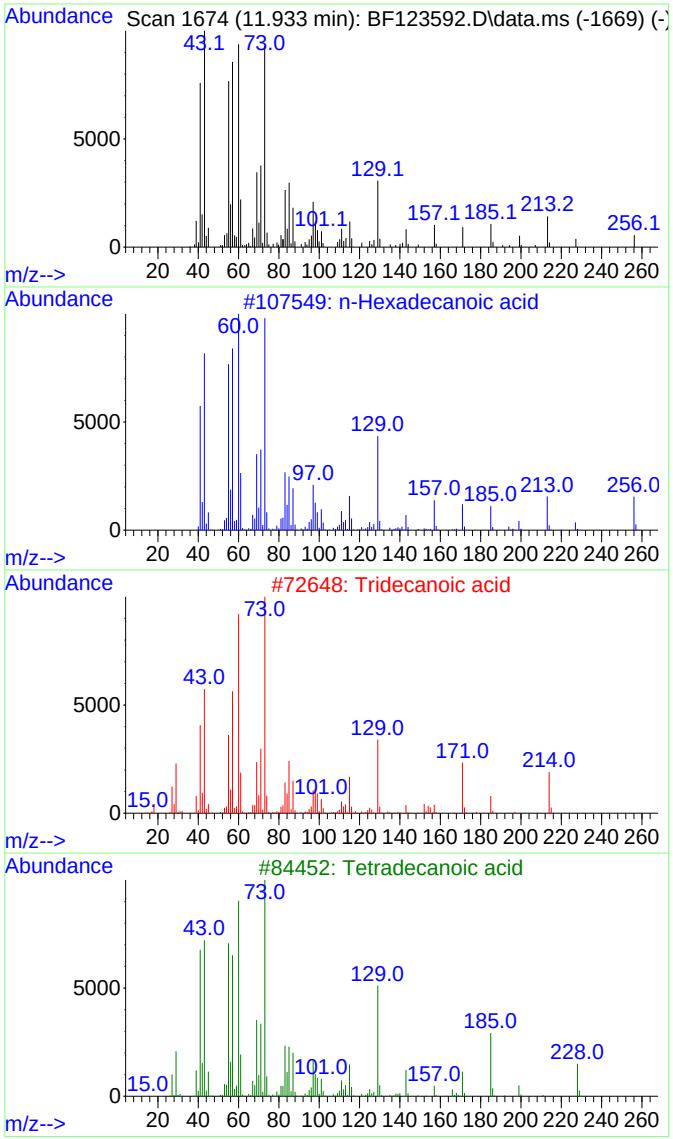
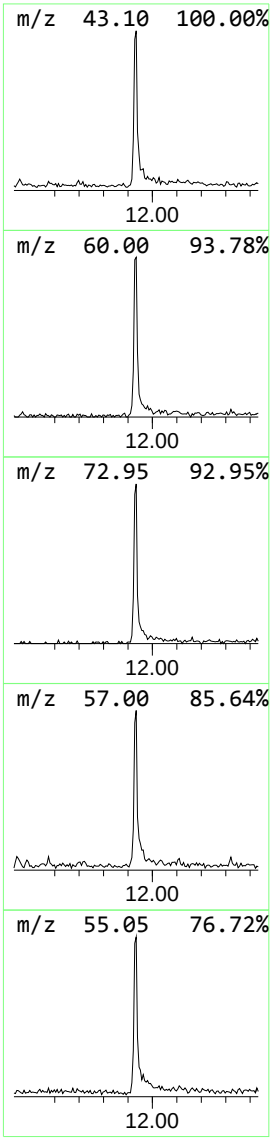
****

Peak Number 2 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.933	4.50 ng	429134	Phenanthrene-d10	11.398

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	81
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	72
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	68
5	Dodecanoic acid	200	C12H24O2	000143-07-7	64





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Instrument :
BNA_F
ClientSampleId :
SB-06-8.5-9.0

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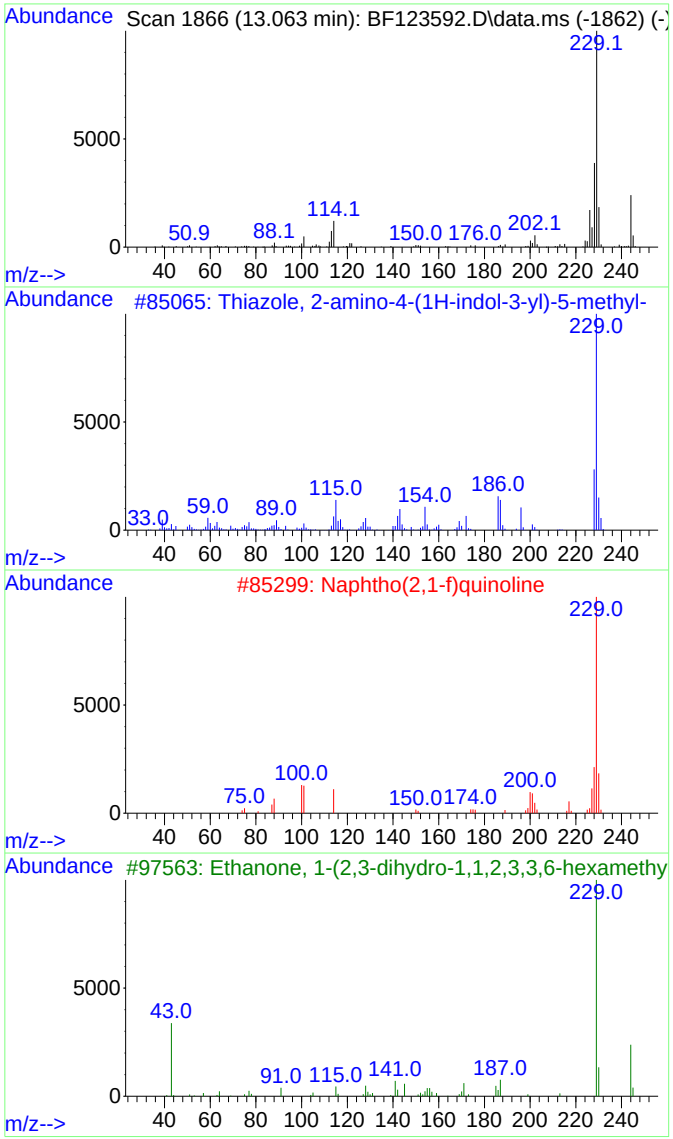
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

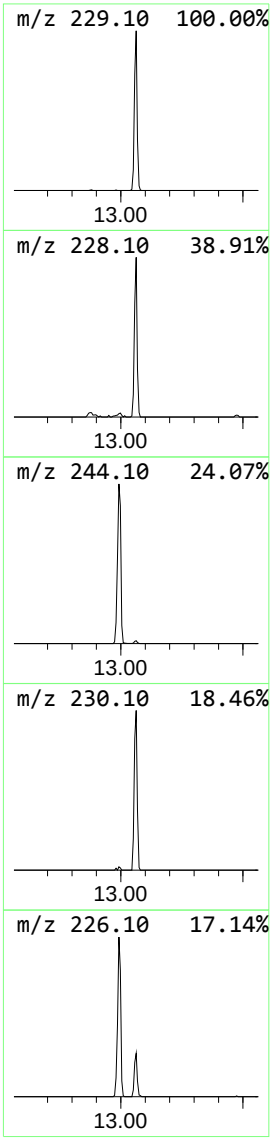
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Thiazole, 2-amino-4-(1H-ind... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.063	4.24 ng	344284	Chrysene-d12	14.045

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Thiazole, 2-amino-4-(1H-indol-3-...	229	C12H11N3S	1000304-18-3	53
2	Naphtho(2,1-f)quinoline	229	C17H11N	000218-08-6	50
3	Ethanone, 1-(2,3-dihydro-1,1,2,3...	244	C17H24O	015323-35-0	47
4	Naphthalene, 2,6-bis(1,1-dimethy...	244	C18H28	042981-76-0	47
5	Tetralin, 6-acetyl-8-isopropyl-2...	244	C17H24O	1000155-43-5	47





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Instrument : BNA_F
ClientSampleId : SB-06-8.5-9.0

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF041521.M
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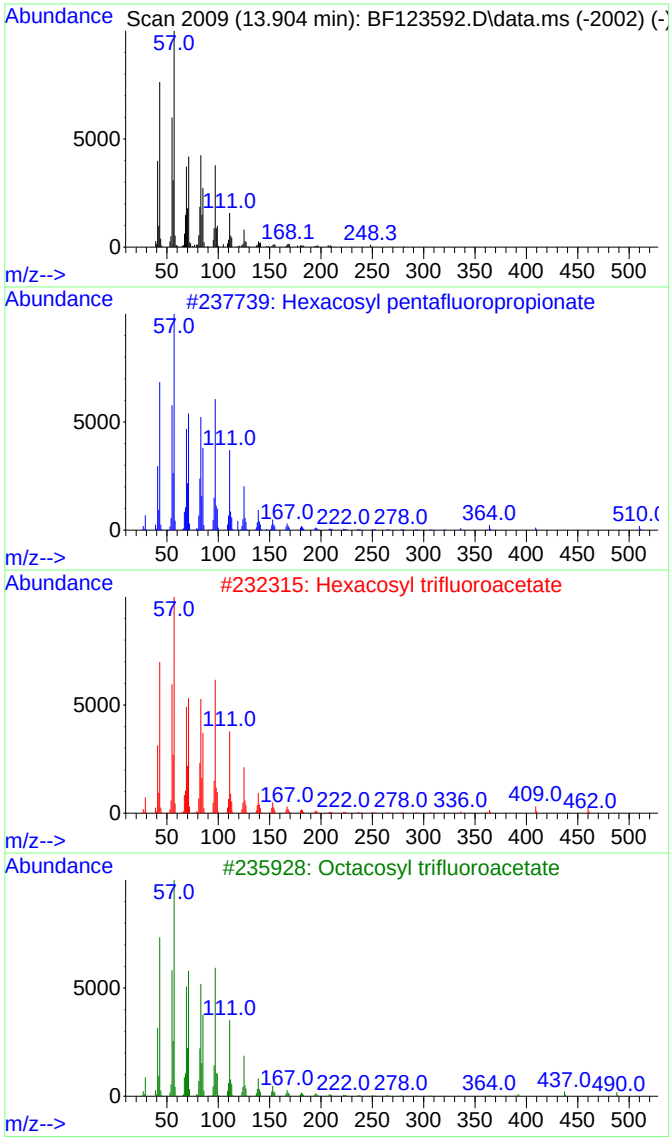
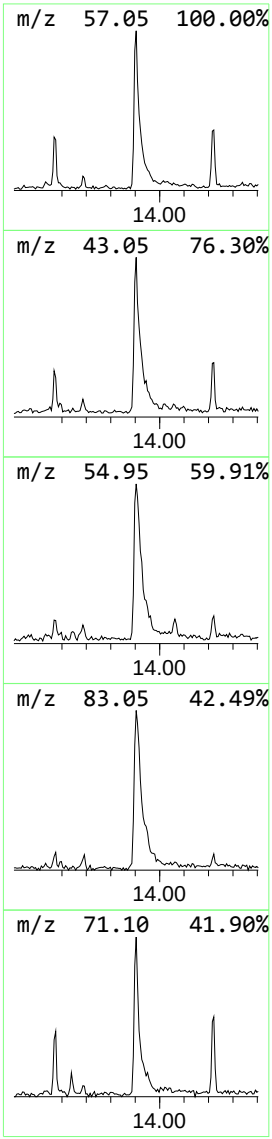
****
Peak Number 4 Hexacosyl pentafluoropropio... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.904	13.84 ng	1123600	Chrysene-d12	14.045

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosyl pentafluoropropionate	528	C29H53F5O2	1000351-81-2	91
2	Hexacosyl trifluoroacetate	478	C28H53F3O2	1000351-75-0	91
3	Octacosyl trifluoroacetate	506	C30H57F3O2	1000351-74-9	91
4	Tricosyl heptafluorobutyrate	536	C27H47F7O2	1000351-83-4	91
5	Tetracosyl heptafluorobutyrate	550	C28H49F7O2	1000351-83-7	91





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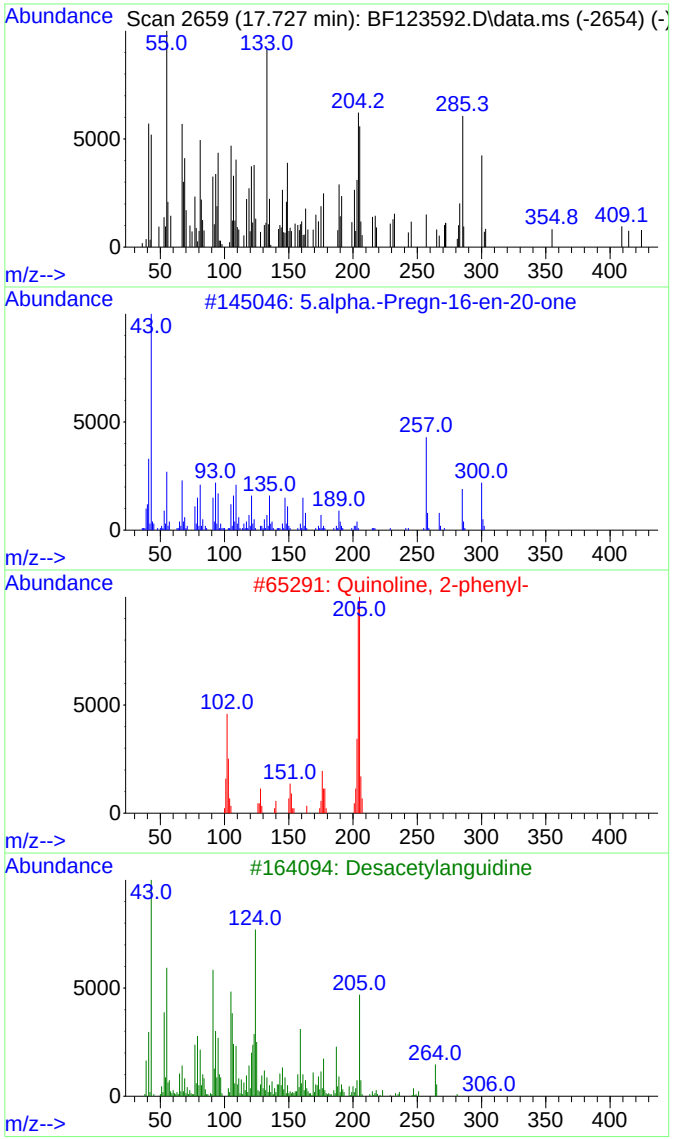
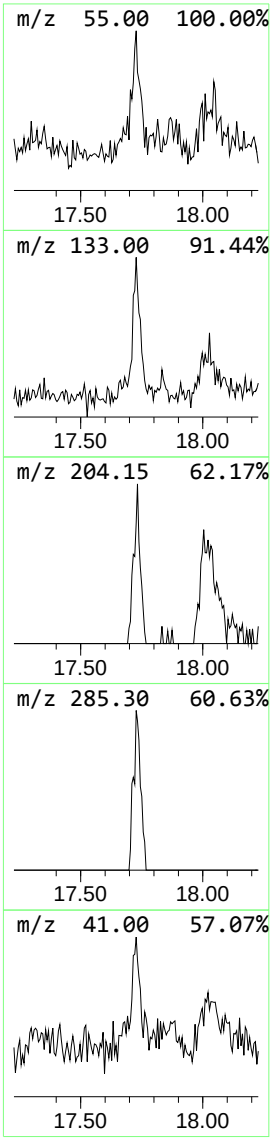
****

Peak Number 5 unknown17.727 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.727	3.35 ng	216017	Perylene-d12	15.533

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5.alpha.-Pregn-16-en-20-one	300	C21H32O	003752-04-3	38
2	Quinoline, 2-phenyl-	205	C15H11N	000612-96-4	25
3	Desacetylanguidine	324	C17H24O6	002623-22-5	18
4	3,4-Dimethylbenzamide	149	C9H11NO	005580-33-6	18
5	4H-1-Benzopyran-4-one, 3,7-dihyd...	300	C16H12O6	057396-72-2	15





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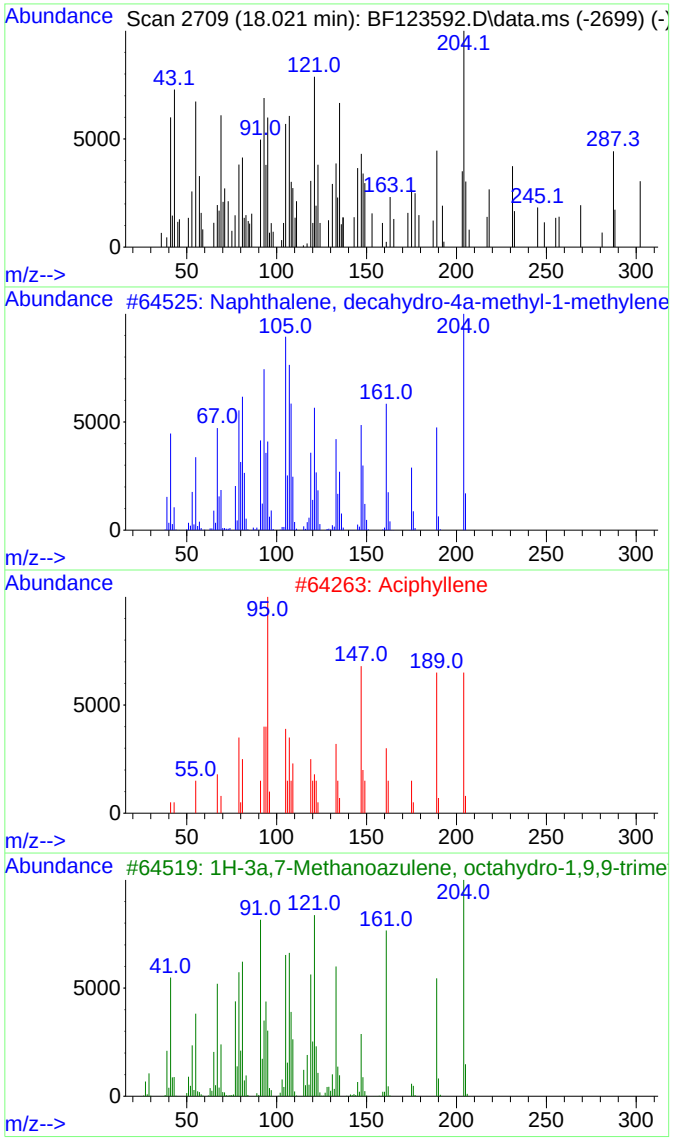
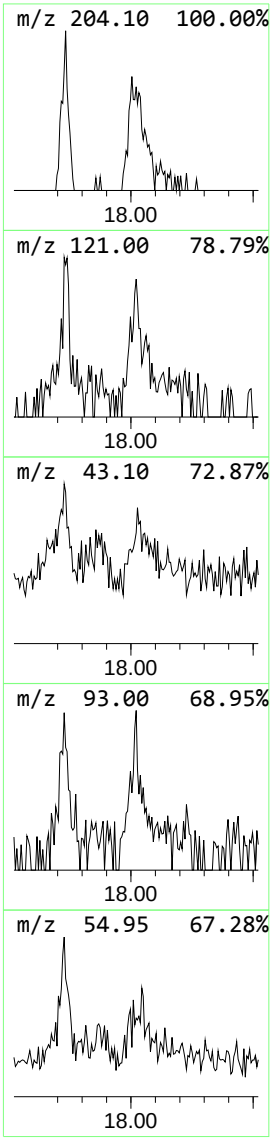
****
Peak Number 6 Naphthalene, decahydro-4a-m... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.021	4.65 ng	300284	Perylene-d12	15.533

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, decahydro-4a-methyl...	204	C15H24	017066-67-0	64
2	Aciphyllene	204	C15H24	087745-31-1	45
3	1H-3a,7-Methanoazulene, octahydr...	204	C15H24	000508-55-4	43
4	1S,2S,5R-1,4,4-Trimethyltricyclo...	204	C15H24	1000140-07-5	42
5	.alpha.-Guaiene	204	C15H24	003691-12-1	42





Tentatively Identified Compound (LSC) summary

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					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Butane, 2-metho...	2.116	33.0	ng	2084330	1	6.869	1264540	20.0
n-Hexadecanoic ...	11.933	4.5	ng	429134	4	11.398	1906410	20.0
Thiazole, 2-ami...	13.063	4.2	ng	344284	5	14.045	1623190	20.0
Hexacosyl penta...	13.904	13.8	ng	1123600	5	14.045	1623190	20.0
unknown17.727	17.727	3.4	ng	216017	6	15.533	1291040	20.0
Naphthalene, de...	18.021	4.7	ng	300284	6	15.533	1291040	20.0