LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM030521\
Data File : BM028999.D
Acq On : 05 Mar 2021 17:03
Operator : CG/JU
Sample : M1553-09
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : 1742

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_M\Methods\8270-BM022321.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM028999.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.245	379	384	396	rBV	112850	162934	31.17%	5.222%
2	6.863	654	659	669	rVB	63687	102705	19.65%	3.291%
3	7.675	792	797	806	rBV	37510	57376	10.98%	1.839%
4	8.851	990	997	1006	rVB	129608	198912	38.05%	6.375%
5	10.469	1265	1272	1279	rVB	46263	74324	14.22%	2.382%
6	12.963	1689	1696	1702	rBV	282716	399541	76.43%	12.804%
7	13.810	1836	1840	1845	rVB	6928	8566	1.64%	0.275%
8	14.345	1926	1931	1937	rBB2	63712	88668	16.96%	2.842%
9	15.845	2180	2186	2192	rVB	275724	363362	69.51%	11.645%
10	17.092	2392	2398	2404	rBV	81569	103090	19.72%	3.304%
11	17.762	2508	2512	2517	rBV2	7292	9085	1.74%	0.291%
12	17.992	2546	2551	2564	rBV	44830	59155	11.32%	1.896%
13	18.468	2627	2632	2639	rVB	5044	8591	1.64%	0.275%
14	18.733	2672	2677	2682	rVB	24075	28065	5.37%	0.899%
15	18.821	2688	2692	2696	rBV	5512	5958	1.14%	0.191%
16	19.209	2753	2758	2763	rBV	405458	423714	81.06%	13.579%
17	19.274	2763	2769	2778	rVV	21194	28341	5.42%	0.908%
18	19.721	2840	2845	2852	rVB	460195	522724	100.00%	16.752%
19	20.121	2909	2913	2916	rBV2	6071	7231	1.38%	0.232%
20	20.215	2923	2929	2935	rBV	64649	76146	14.57%	2.440%
21	20.980	3055	3059	3065	rBV	72660	91766	17.56%	2.941%
22	21.268	3103	3108	3114	rBV	111675	131827	25.22%	4.225%
23	23.432	3470	3476	3483	rVB2	80731	138273	26.45%	4.431%
24	24.009	3569	3574	3582	rVB7	13557	29999	5.74%	0.961%

Sum of corrected areas: 3120353

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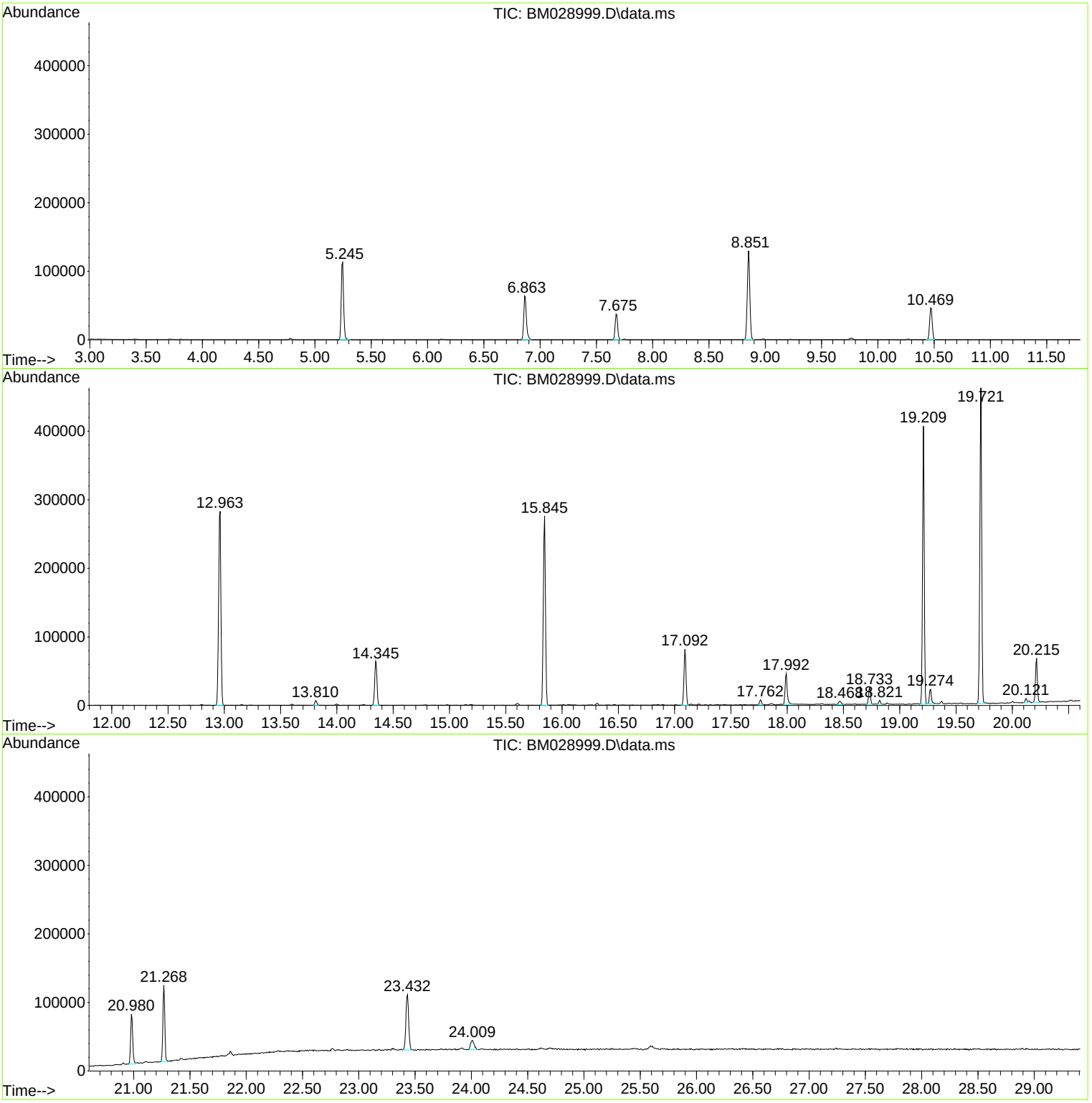
ClientSampleId :
1742

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM022321.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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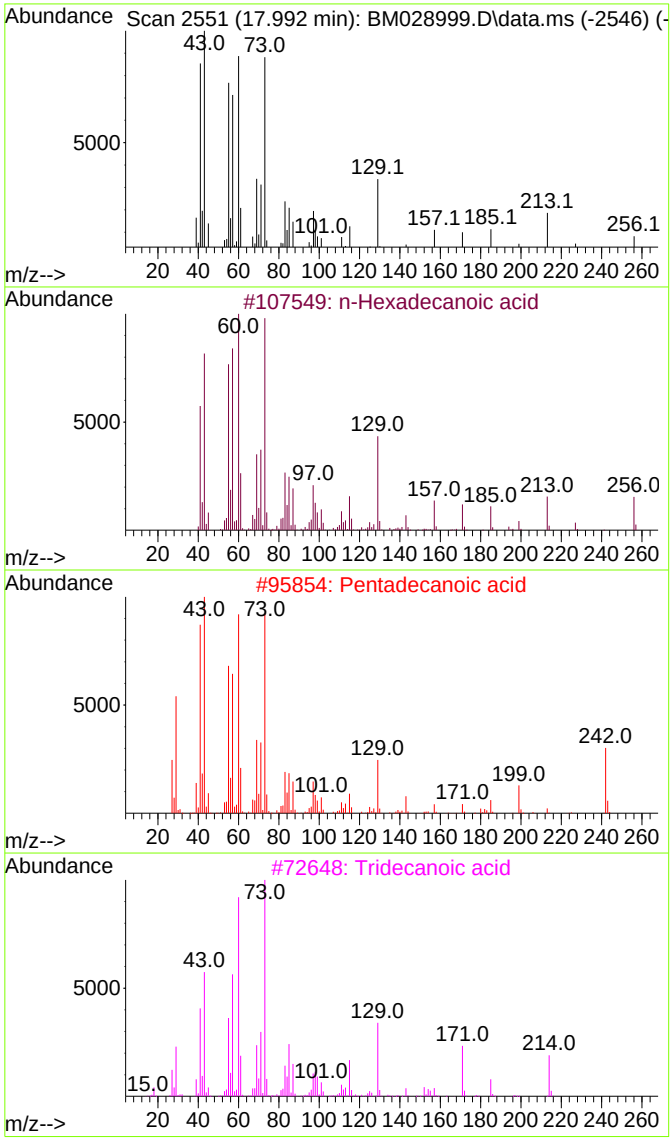
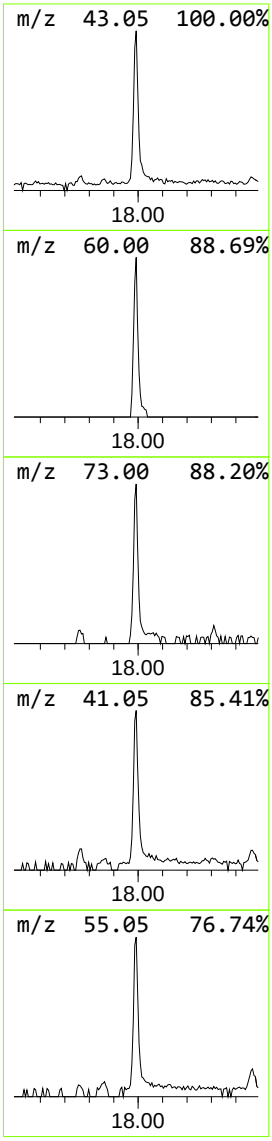
****

Peak Number 1 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.992	11.48 ng	59155	Phenanthrene-d10	17.092

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
3	Tridecanoic acid	214	C13H26O2	000638-53-9	72
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	72
5	Undecanoic acid	186	C11H22O2	000112-37-8	59





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Instrument : BNA_M
ClientSampleId : 1742

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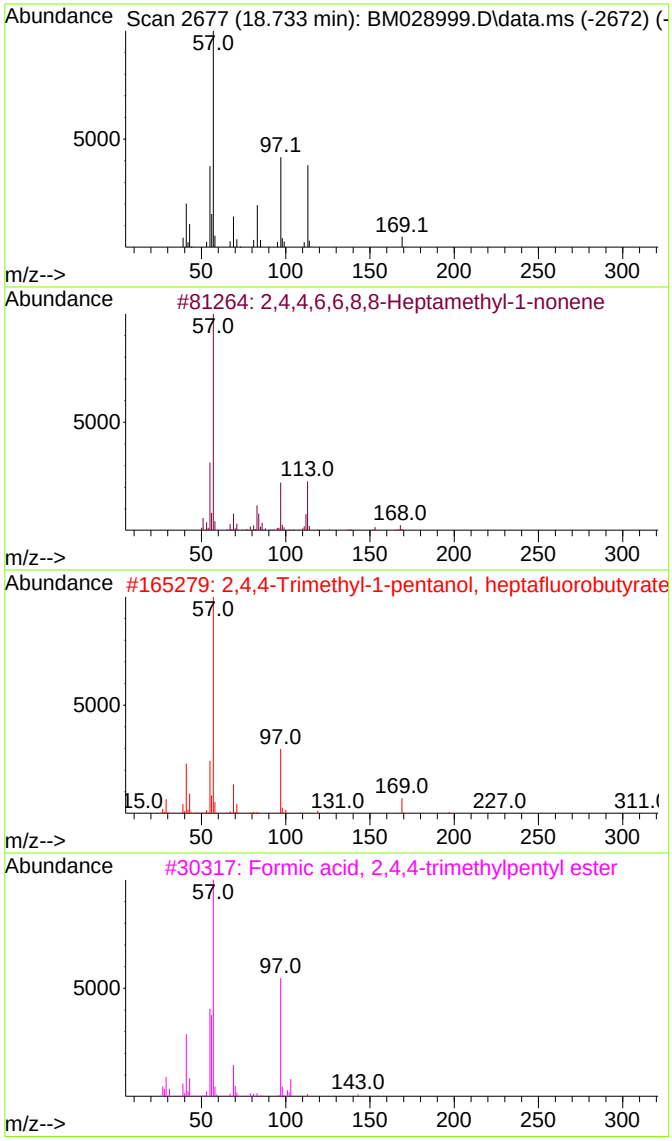
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

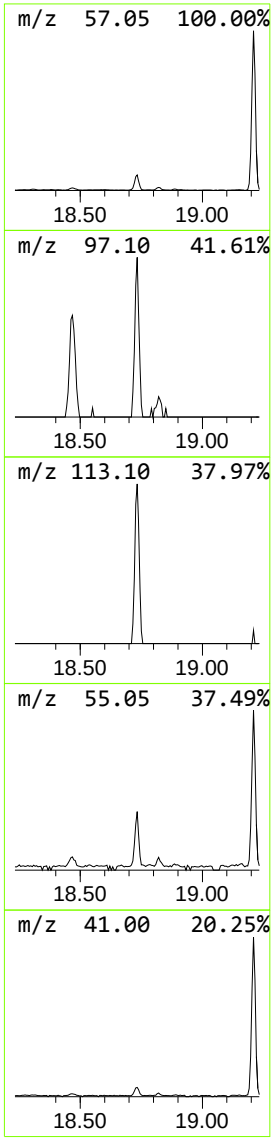
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 2,4,4,6,6,8,8-Heptamethyl-1... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.733	5.44 ng	28065	Phenanthrene-d10	17.092

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4,4,6,6,8,8-Heptamethyl-1-nonene	224	C16H32	015796-04-0	78
2	2,4,4-Trimethyl-1-pentanol, hept...	326	C12H17F7O2	1000365-01-4	47
3	Formic acid, 2,4,4-trimethylpent...	158	C9H18O2	1000368-95-2	37
4	Octane, 2-bromo-	192	C8H17Br	000557-35-7	35
5	Sulfurous acid, butyl heptadecyl...	376	C21H44O3S	1000309-18-4	28





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Operator : CG/JU
Sample : M1553-09
Misc :
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Instrument : BNA_M
ClientSampleId : 1742

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM022321.M
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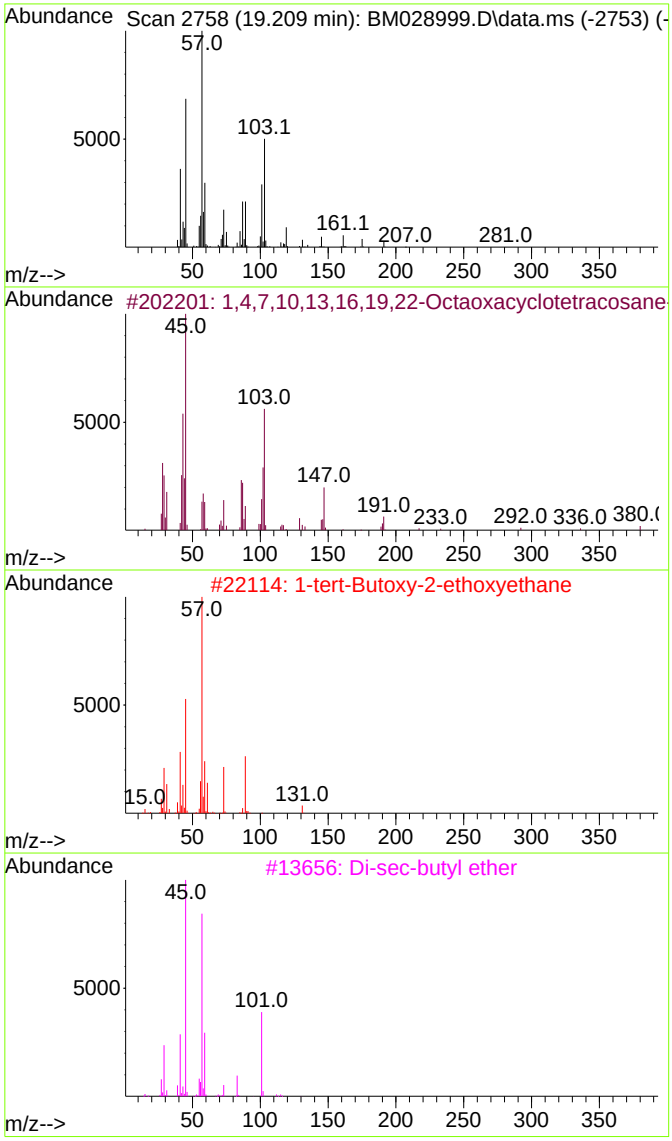
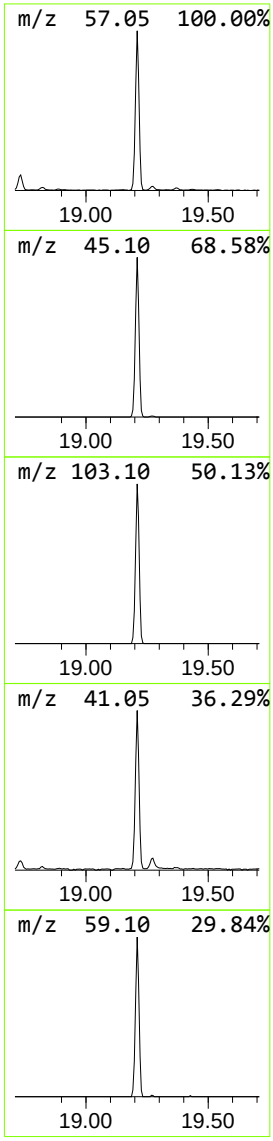
****
Peak Number 3 1,4,7,10,13,16,19,22-Octaox... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.209	64.28 ng	423714	Chrysene-d12	21.268

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,4,7,10,13,16,19,22-Octaoxacycl...	380	C16H28O10	1000221-60-1	53
2	1-tert-Butoxy-2-ethoxyethane	146	C8H18O2	051422-54-9	43
3	Di-sec-butyl ether	130	C8H18O	006863-58-7	38
4	3,6,9,12-Tetraoxatetradecan-1-ol	222	C10H22O5	005650-20-4	35
5	Butane, 1-(1-methylpropoxy)-	130	C8H18O	000999-65-5	35





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Sample : M1553-09
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : 1742

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM022321.M
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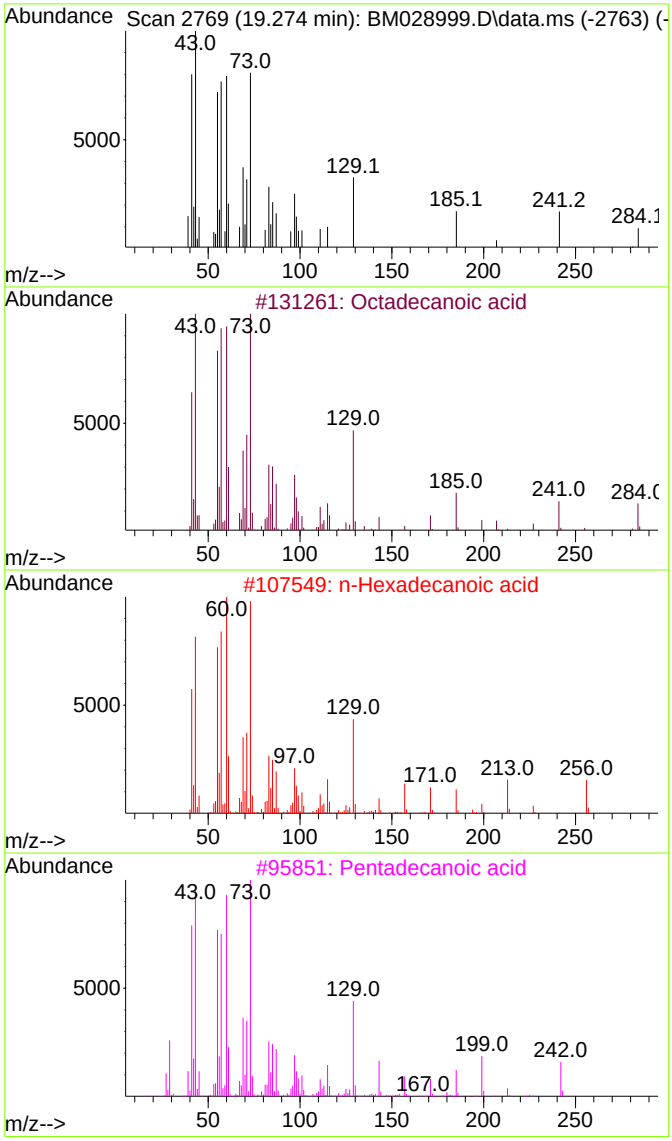
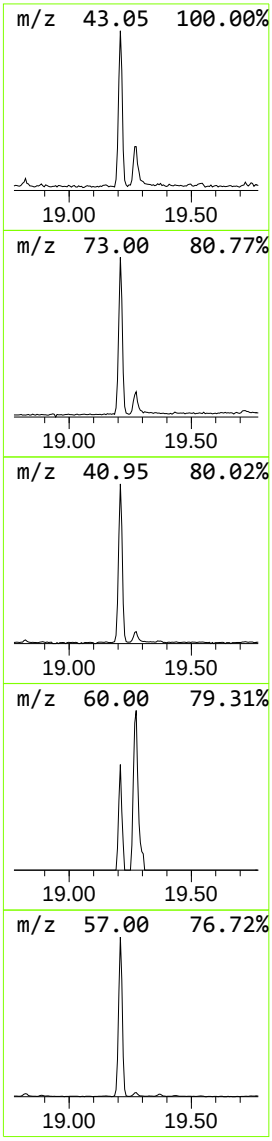
Peak Number 4 Octadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.274	4.30 ng	28341	Chrysene-d12	21.268

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	97
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	83
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	83
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	80
5	Tridecanoic acid	214	C13H26O2	000638-53-9	72





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Sample : M1553-09
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Instrument : BNA_M
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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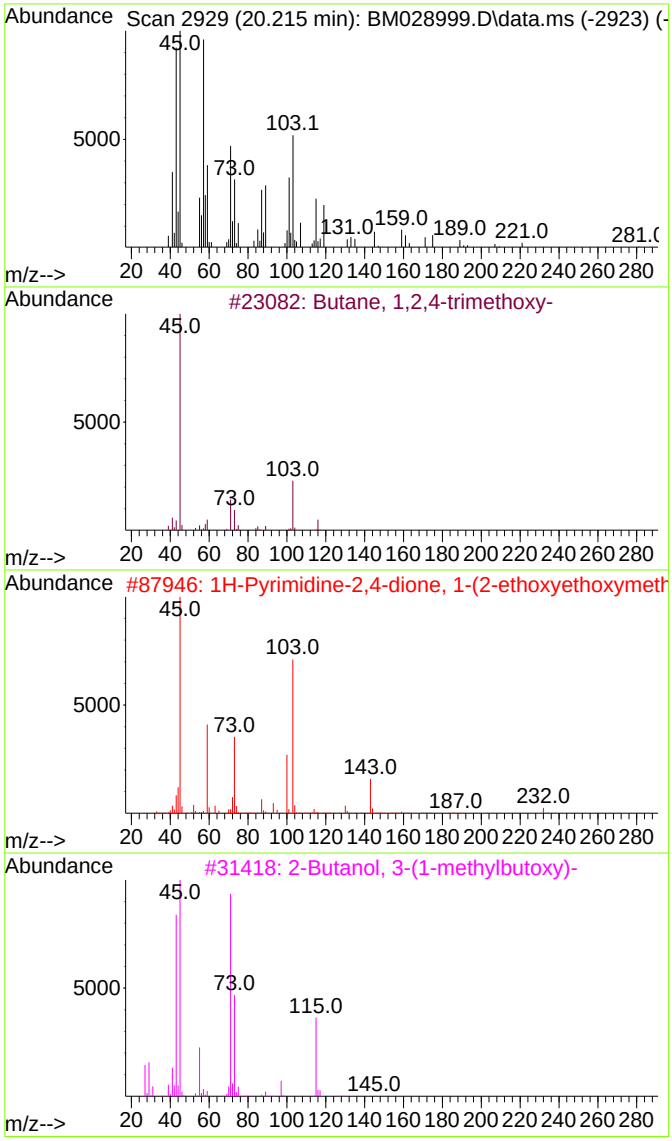
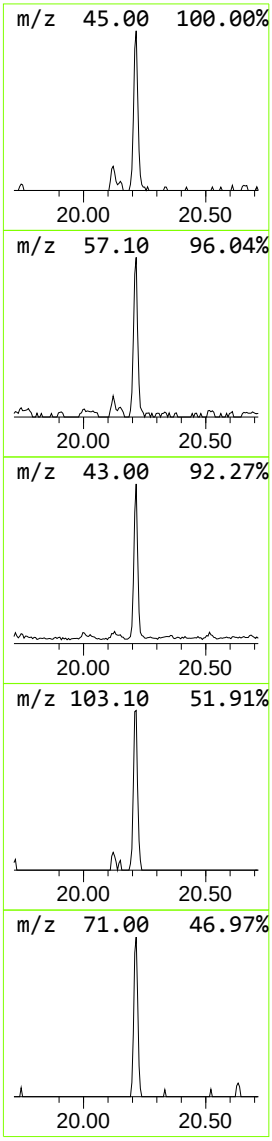
Peak Number 5 unknown20.21 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.215	11.55 ng	76146	Chrysene-d12	21.268

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 1,2,4-trimethoxy-	148	C7H16O3	020637-48-3	47
2	1H-Pyrimidine-2,4-dione, 1-(2-et...	232	C9H13FN2O4	1000310-13-7	43
3	2-Butanol, 3-(1-methylbutoxy)-	160	C9H20O2	074810-43-8	38
4	3,6,9,12,15-Pentaoxanonadecan-1-ol	294	C14H30O6	001786-94-3	35
5	2-Propanol, 1-(1-methylethoxy)-	118	C6H14O2	003944-36-3	35





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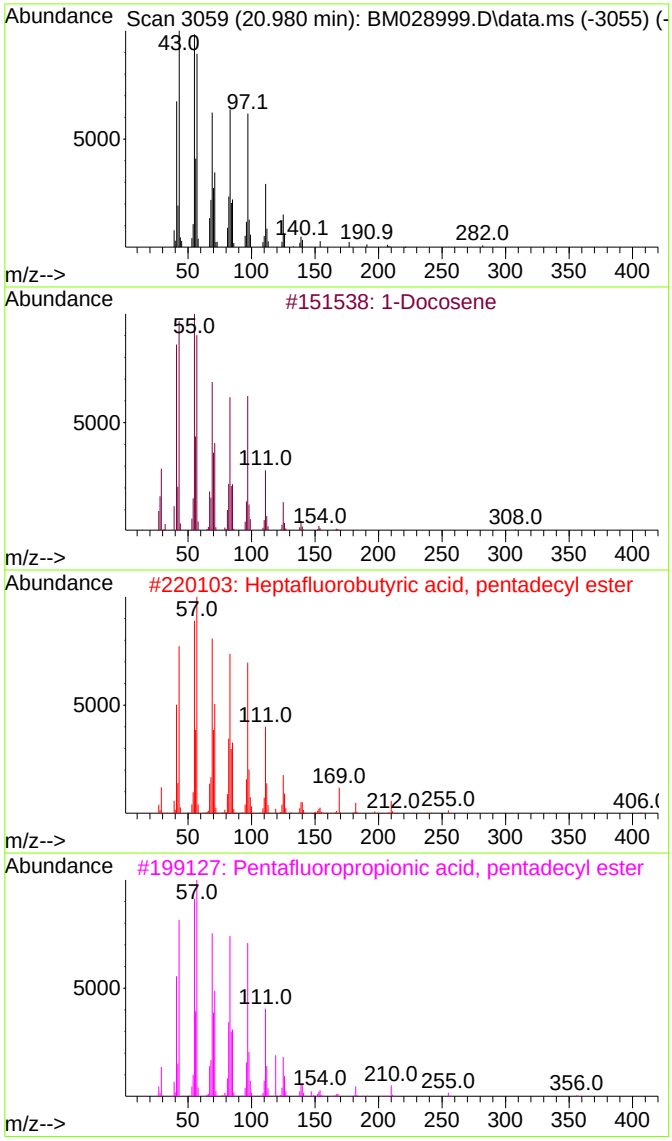
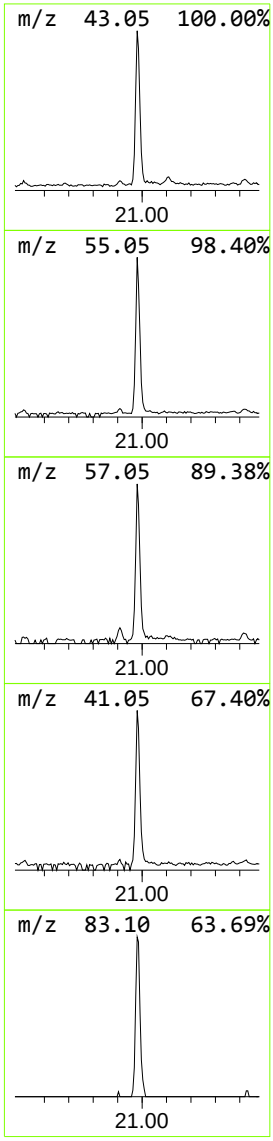
Peak Number 6 1-Docosene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.980	13.92 ng	91766	Chrysene-d12	21.268

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Docosene	308	C22H44	001599-67-3	95
2	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	93
3	Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	93
4	Pentafluoropropionic acid, hexad...	388	C19H33F5O2	006222-07-7	91
5	1-Octadecanol	270	C18H38O	000112-92-5	91





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Instrument : BNA_M
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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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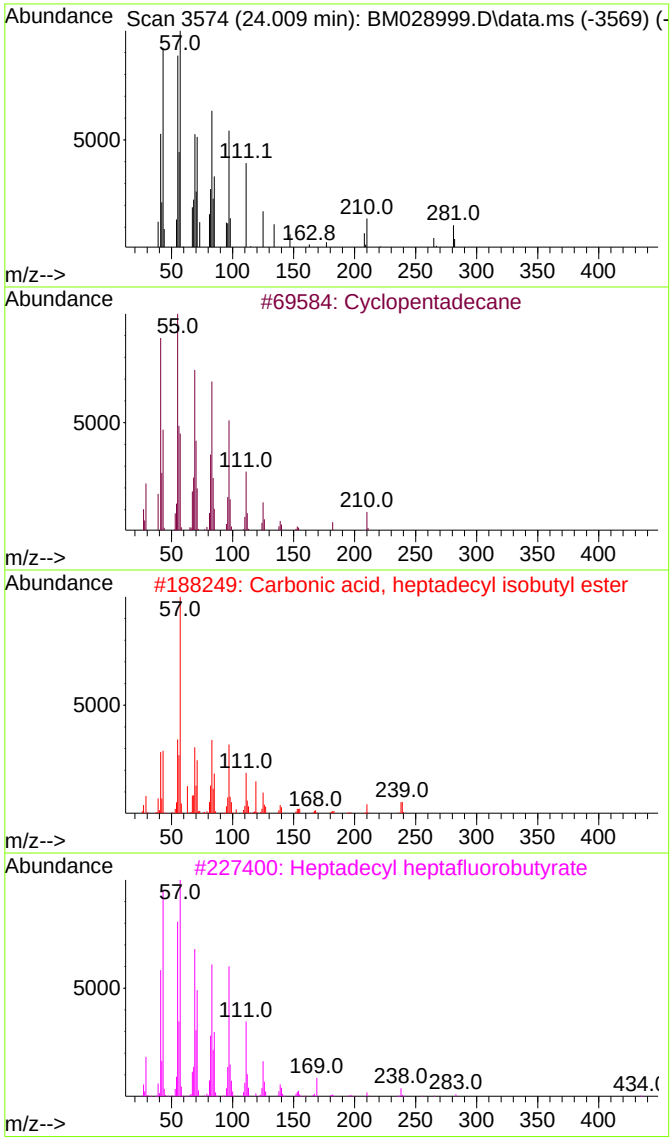
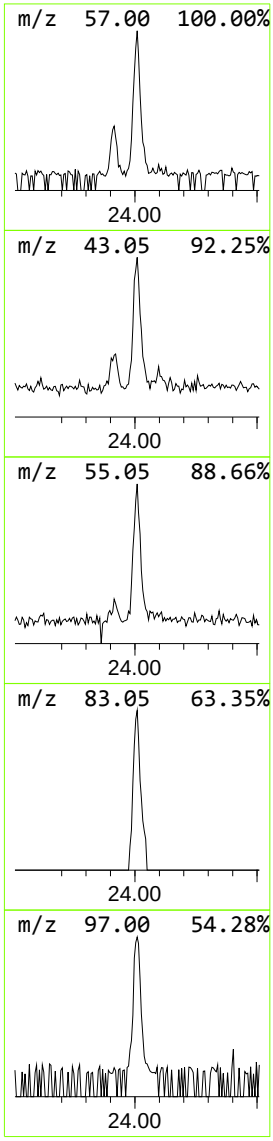
Peak Number 7 Cyclopentadecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.009	4.34 ng	29999	Perylene-d12	23.433

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentadecane	210	C15H30	000295-48-7	95
2	Carbonic acid, heptadecyl isobut...	356	C22H44O3	1000314-61-4	91
3	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	90
4	Heptafluorobutyric acid, hexadec...	438	C20H33F7O2	006385-15-5	90
5	Heptafluorobutyric acid, n-octad...	466	C22H37F7O2	000400-57-7	87





Tentatively Identified Compound (LSC) summary

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TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
n-Hexadecanoic ...	17.992	11.5	ng	59155	4	17.092	103090	20.0
2,4,4,6,6,8,8-H...	18.733	5.4	ng	28065	4	17.092	103090	20.0
1,4,7,10,13,16,...	19.209	64.3	ng	423714	5	21.268	131827	20.0
Octadecanoic acid	19.274	4.3	ng	28341	5	21.268	131827	20.0
unknown20.21	20.215	11.6	ng	76146	5	21.268	131827	20.0
1-Docosene	20.980	13.9	ng	91766	5	21.268	131827	20.0
Cyclopentadecane	24.009	4.3	ng	29999	6	23.433	138273	20.0