LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM030821\
Data File : BM029033.D
Acq On : 08 Mar 2021 23:46
Operator : CG/JU
Sample : M1591-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : FK-PS-01-070

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: BM029033.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	394	rBB	186070	260556	55.63%	8.378%
2	6.869	654	660	671	rBV	174595	267509	57.12%	8.602%
3	7.669	791	796	802	rBB	43759	61731	13.18%	1.985%
4	8.845	989	996	1008	rVB	105081	170517	36.41%	5.483%
5	10.463	1265	1271	1277	rBV	49013	78260	16.71%	2.517%
6	12.951	1688	1694	1702	rBB	243909	332981	71.10%	10.707%
7	14.221	1902	1910	1920	rBV4	5357	14166	3.02%	0.456%
8	14.339	1924	1930	1937	rVB	66369	95224	20.33%	3.062%
9	15.833	2179	2184	2192	rBV	179175	244673	52.24%	7.868%
10	17.080	2391	2396	2400	rBV	77831	104603	22.33%	3.364%
11	17.121	2400	2403	2409	rVB	36590	47681	10.18%	1.533%
12	17.215	2415	2419	2424	rVB	9806	11716	2.50%	0.377%
13	17.980	2541	2549	2559	rBV2	32749	52667	11.25%	1.694%
14	18.150	2572	2578	2582	rBV3	6055	9480	2.02%	0.305%
15	19.139	2740	2746	2751	rBV	52992	69662	14.87%	2.240%
16	19.262	2763	2767	2771	rBV3	11672	13971	2.98%	0.449%
17	19.503	2798	2808	2812	rBV	44487	68372	14.60%	2.199%
18	19.709	2836	2843	2848	rBV	394712	468342	100.00%	15.060%
19	19.833	2858	2864	2869	rBV5	3026	6912	1.48%	0.222%
20	20.003	2882	2893	2898	rBV4	10354	22678	4.84%	0.729%
21	20.097	2906	2909	2913	rVB	6795	7491	1.60%	0.241%
22	20.156	2915	2919	2923	rVV2	3934	5894	1.26%	0.190%
23	20.344	2948	2951	2955	rBV4	9043	11327	2.42%	0.364%
24	20.509	2976	2979	2982	rVB3	5628	6719	1.43%	0.216%
25	20.944	3050	3053	3054	rBV2	6562	6346	1.35%	0.204%
26	20.974	3054	3058	3065	rVB2	62401	84949	18.14%	2.732%
27	21.256	3100	3106	3110	rBV2	124979	184850	39.47%	5.944%
28	21.291	3110	3112	3121	rVB	28168	32887	7.02%	1.058%
29	21.403	3128	3131	3136	rBV4	11387	18554	3.96%	0.597%
30	21.821	3200	3202	3203	rBV	11913	10132	2.16%	0.326%
31	21.844	3203	3206	3212	rVB2	33352	44578	9.52%	1.433%
32	22.750	3355	3360	3363	rBV	41589	69571	14.85%	2.237%
33	23.321	3454	3457	3467	rVB	22293	35787	7.64%	1.151%
34	23.415	3467	3473	3479	rBV2	78502	146645	31.31%	4.716%
35	23.891	3551	3554	3561	rVB	25284	42413	9.06%	1.364%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM030821\
Data File : BM029033.D
Acq On : 08 Mar 2021 23:46
Operator : CG/JU
Sample : M1591-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
FK-PS-01-070

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

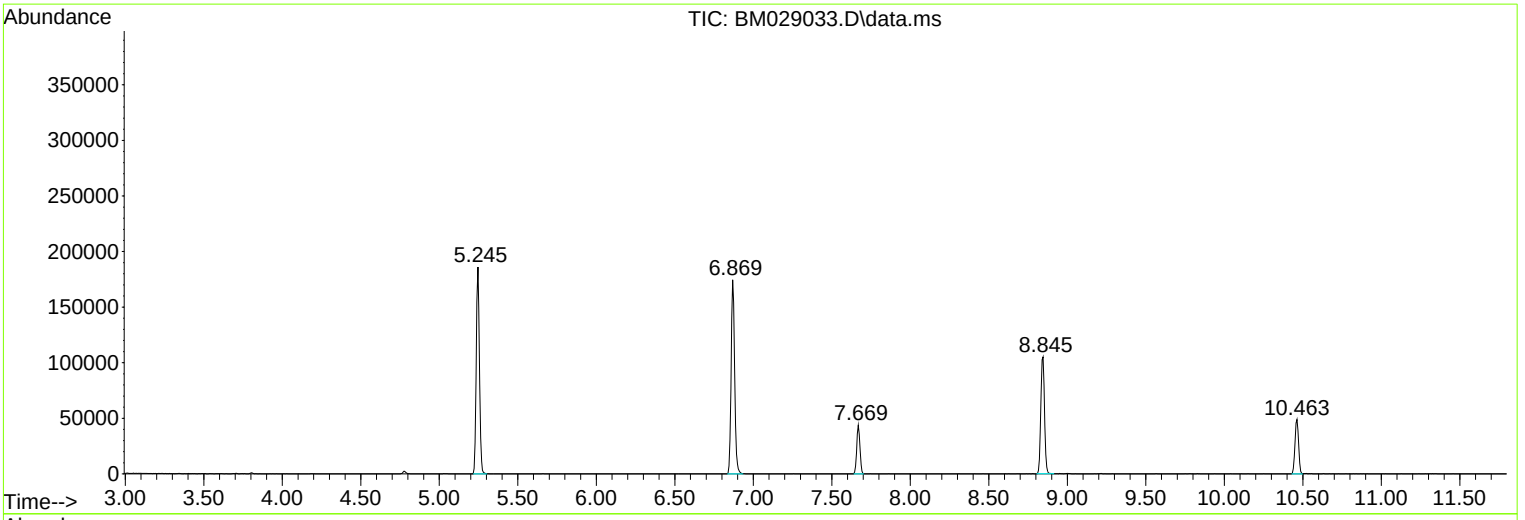
Sum of corrected areas: 3109844

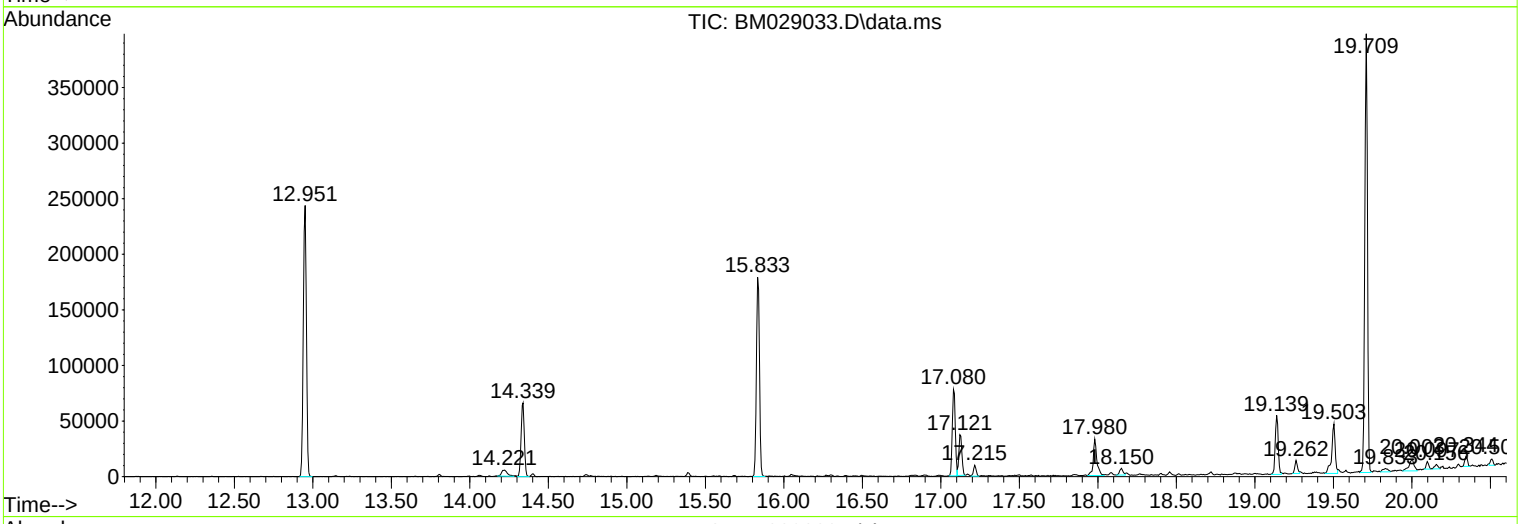
Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM030821\
Data File : BM029033.D
Acq On : 08 Mar 2021 23:46
Operator : CG/JU
Sample : M1591-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

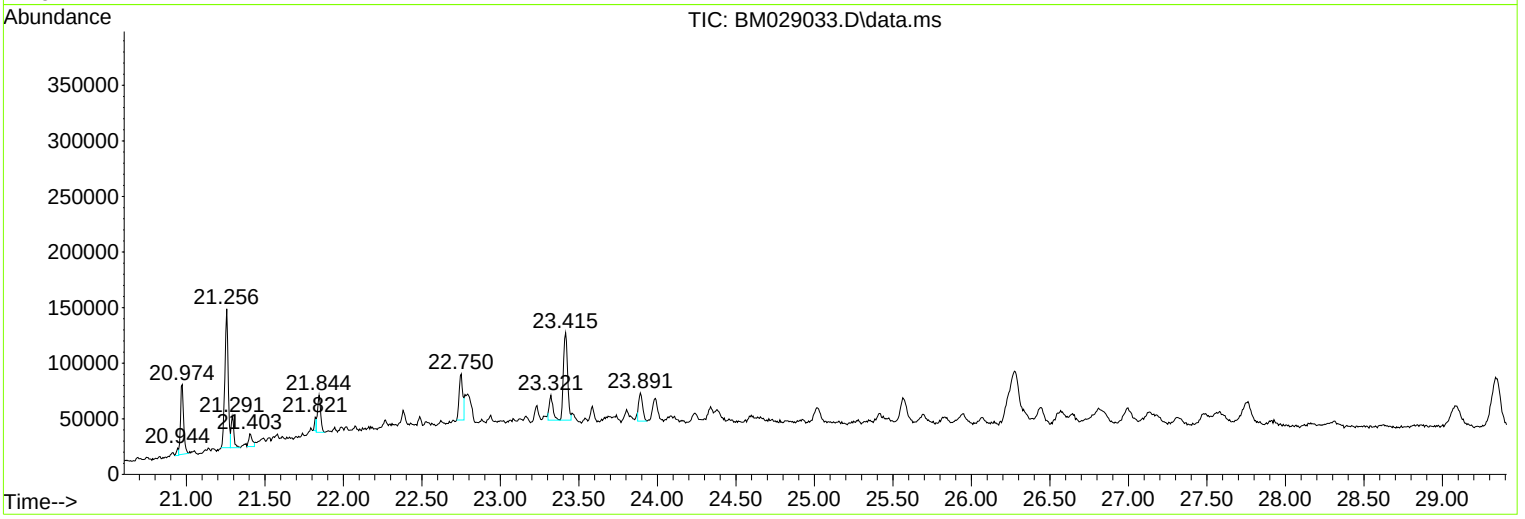
Instrument :
BNA_M
ClientSampleId :
FK-PS-01-070

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







Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM030821\
Data File : BM029033.D
Acq On : 08 Mar 2021 23:46
Operator : CG/JU
Sample : M1591-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
FK-PS-01-070

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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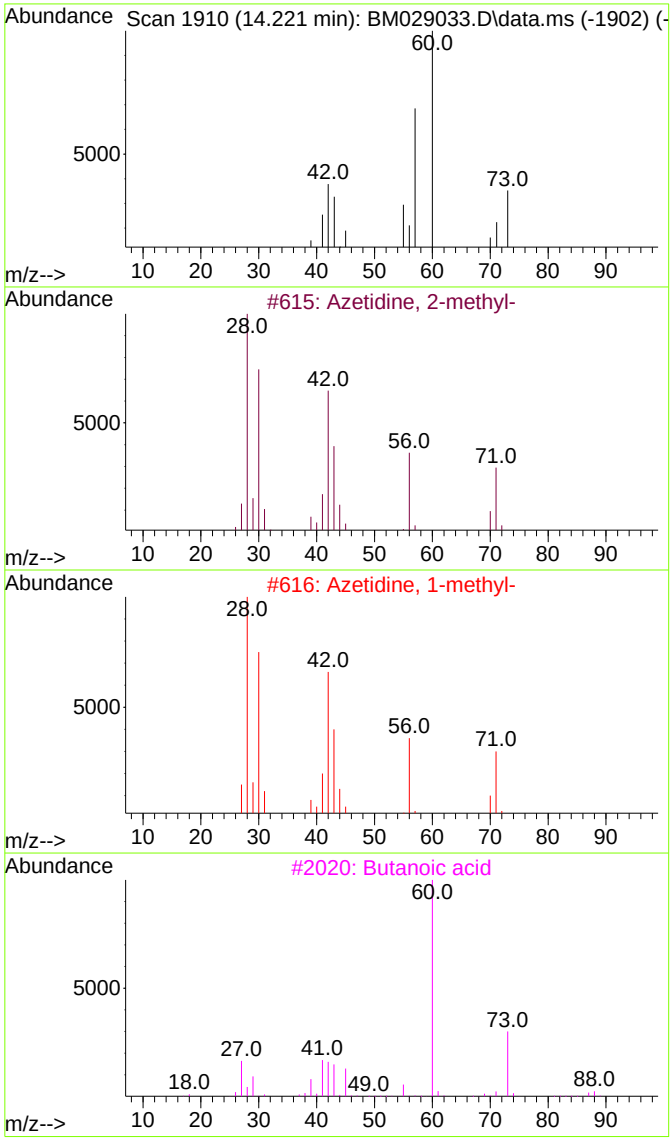
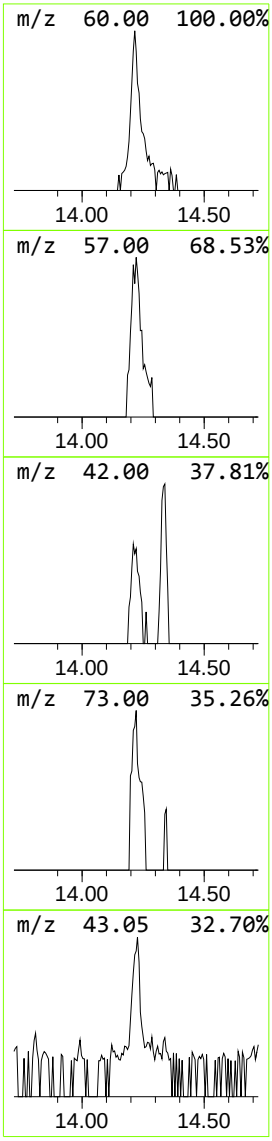
Peak Number 1 unknown14.221 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.221	2.98 ng	14166	Acenaphthene-d10	14.333

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Azetidine, 2-methyl-	71	C4H9N	019812-49-8	12
2	Azetidine, 1-methyl-	71	C4H9N	004923-79-9	12
3	Butanoic acid	88	C4H8O2	000107-92-6	9
4	Hydrazine, 1,1-dimethyl-	60	C2H8N2	000057-14-7	7
5	Aziridine, 2,2-dimethyl-	71	C4H9N	002658-24-4	7





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM030821\
Data File : BM029033.D
Acq On : 08 Mar 2021 23:46
Operator : CG/JU
Sample : M1591-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : FK-PS-01-070

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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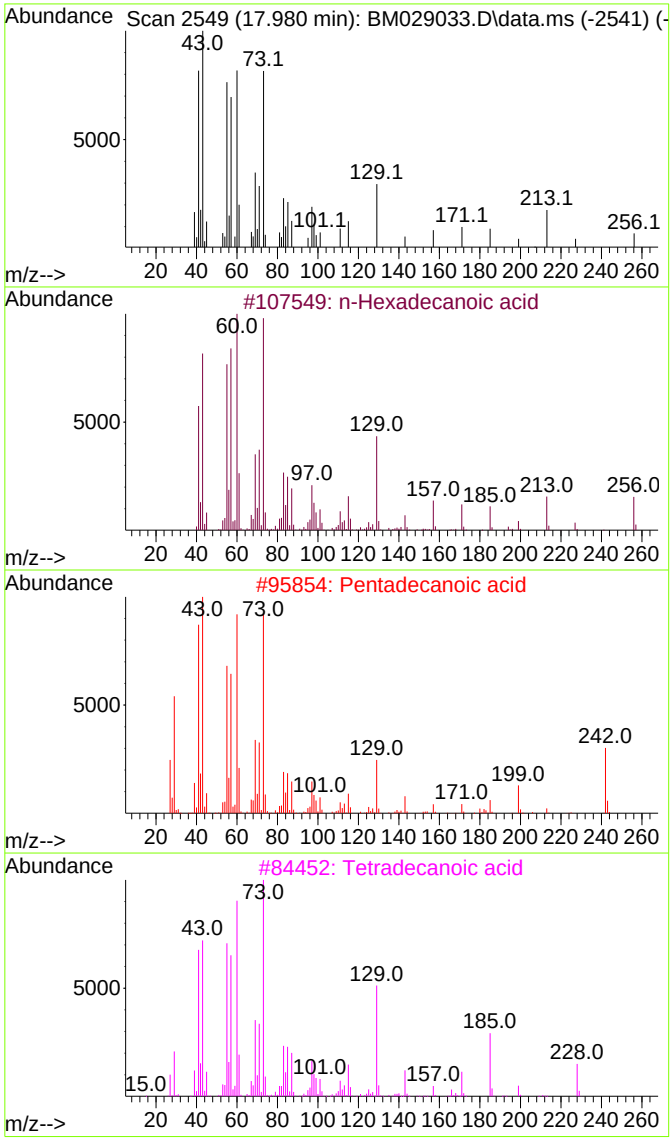
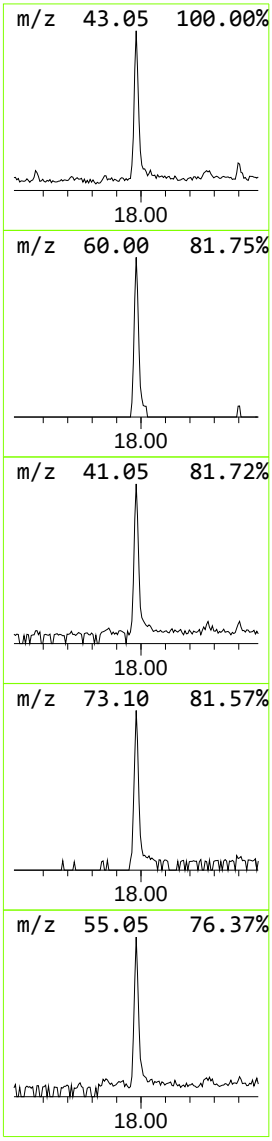
Peak Number 2 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.980	10.07 ng	52667	Phenanthrene-d10	17.080

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	80
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	80
4	Tridecanoic acid	214	C13H26O2	000638-53-9	72
5	n-Decanoic acid	172	C10H20O2	000334-48-5	47





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM030821\
Data File : BM029033.D
Acq On : 08 Mar 2021 23:46
Operator : CG/JU
Sample : M1591-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
FK-PS-01-070

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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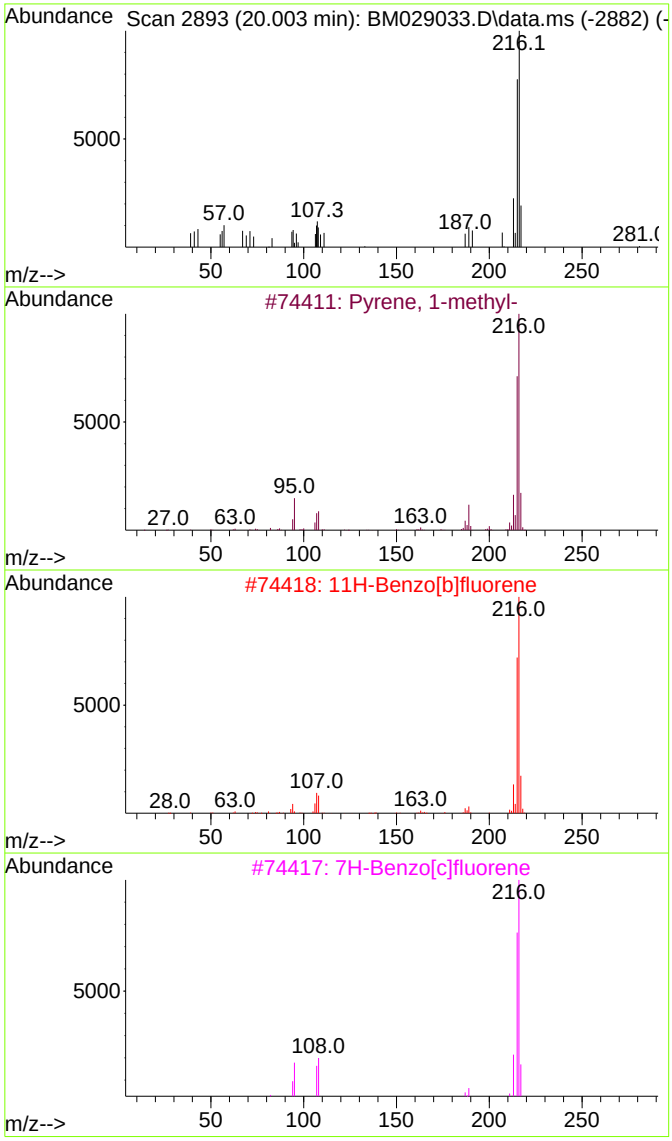
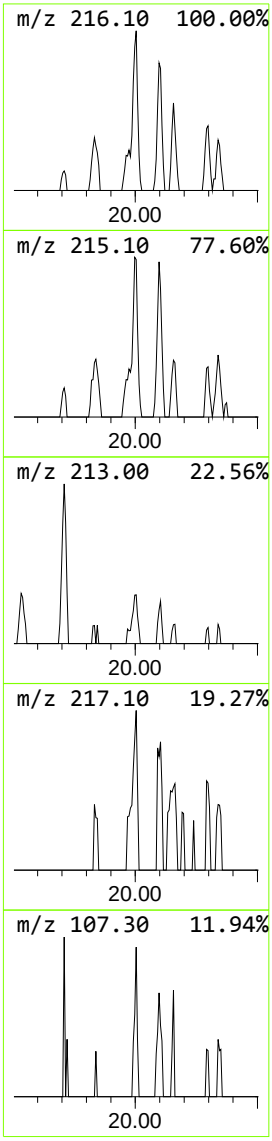
Peak Number 3 Pyrene, 1-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.003	2.45 ng	22678	Chrysene-d12	21.256

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pyrene, 1-methyl-	216	C17H12	002381-21-7	87
2	11H-Benzo[b]fluorene	216	C17H12	000243-17-4	87
3	7H-Benzo[c]fluorene	216	C17H12	000205-12-9	72
4	Fluoranthene, 2-methyl-	216	C17H12	033543-31-6	64
5	11H-Benzo[a]fluorene	216	C17H12	000238-84-6	64





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM030821\
Data File : BM029033.D
Acq On : 08 Mar 2021 23:46
Operator : CG/JU
Sample : M1591-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
FK-PS-01-070

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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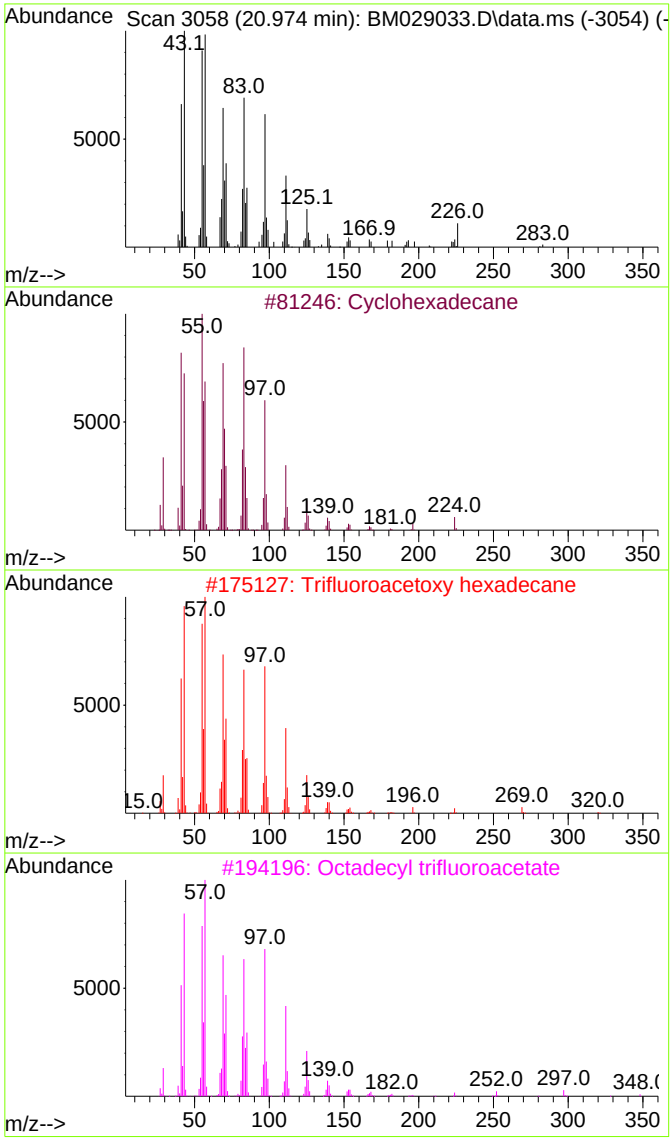
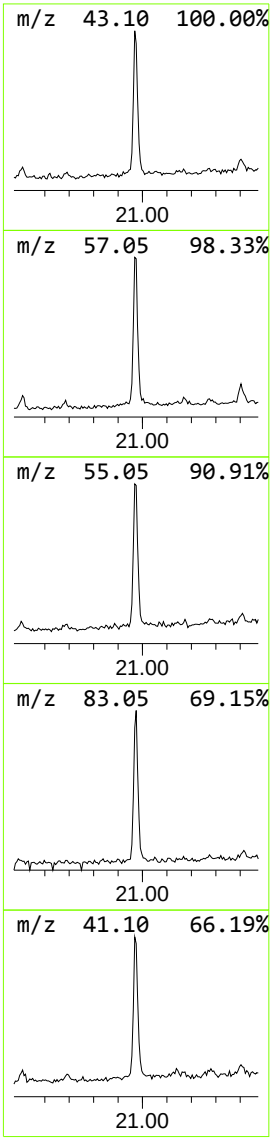
Peak Number 4 Cyclohexadecane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.974	9.19 ng	84949	Chrysene-d12	21.256

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexadecane	224	C16H32	000295-65-8	96
2	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	95
3	Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	95
4	Pentafluoropropionic acid, hexad...	388	C19H33F5O2	006222-07-7	95
5	Heptafluorobutyric acid, hexadec...	438	C20H33F7O2	006385-15-5	94





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM030821\
Data File : BM029033.D
Acq On : 08 Mar 2021 23:46
Operator : CG/JU
Sample : M1591-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
FK-PS-01-070

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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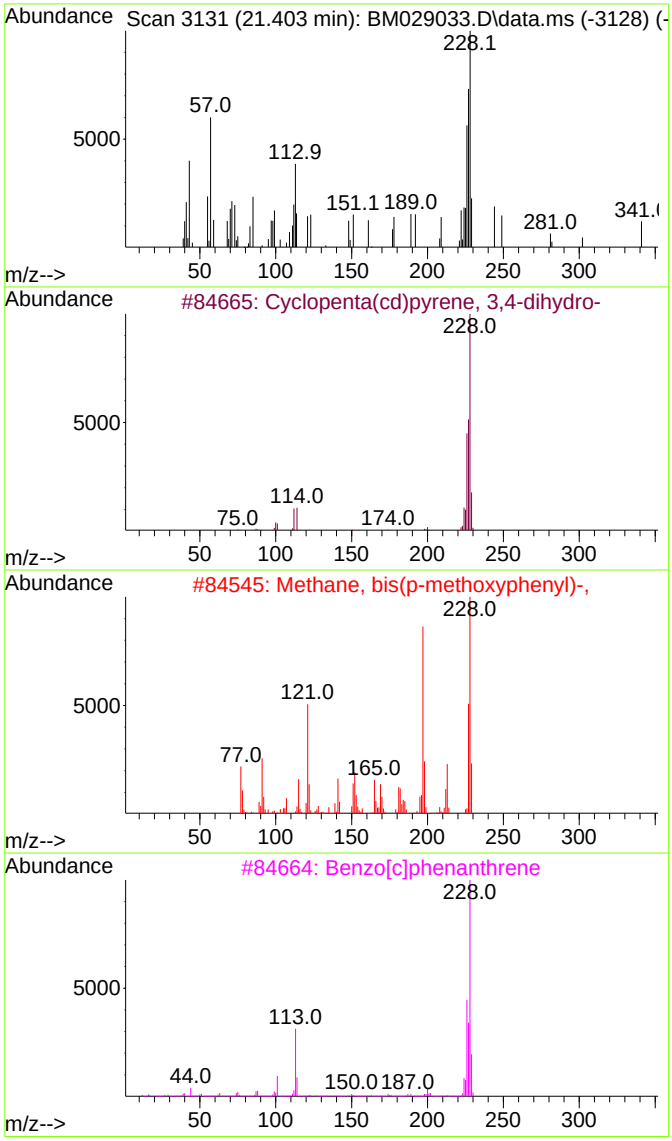
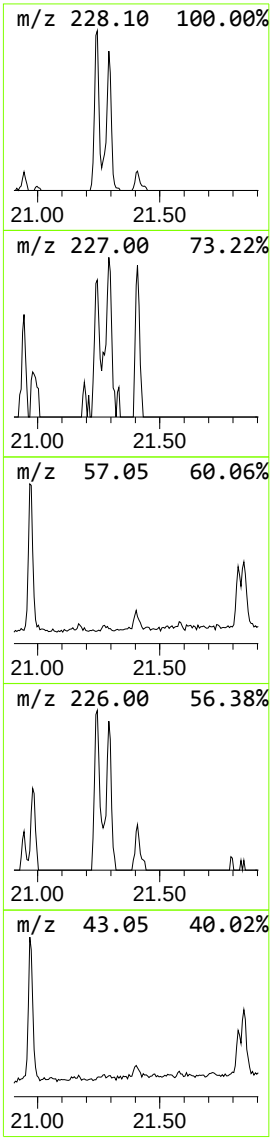
Peak Number 5 unknown21.403 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.403	2.01 ng	18554	Chrysene-d12	21.256

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopenta(cd)pyrene, 3,4-dihydro-	228	C18H12	025732-74-5	46
2	Methane, bis(p-methoxyphenyl)-,	228	C15H16O2	000726-18-1	43
3	Benzo[c]phenanthrene	228	C18H12	000195-19-7	38
4	2,1,3-Benzoselenadiazole-5-carbo...	228	C7H4N2O2Se	140669-75-6	30
5	Isothiazol-5-amine, 4-bromo-3-ch...	226	C4H4BrClN2S	1000272-59-9	27





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Acq On : 08 Mar 2021 23:46
Operator : CG/JU
Sample : M1591-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : FK-PS-01-070

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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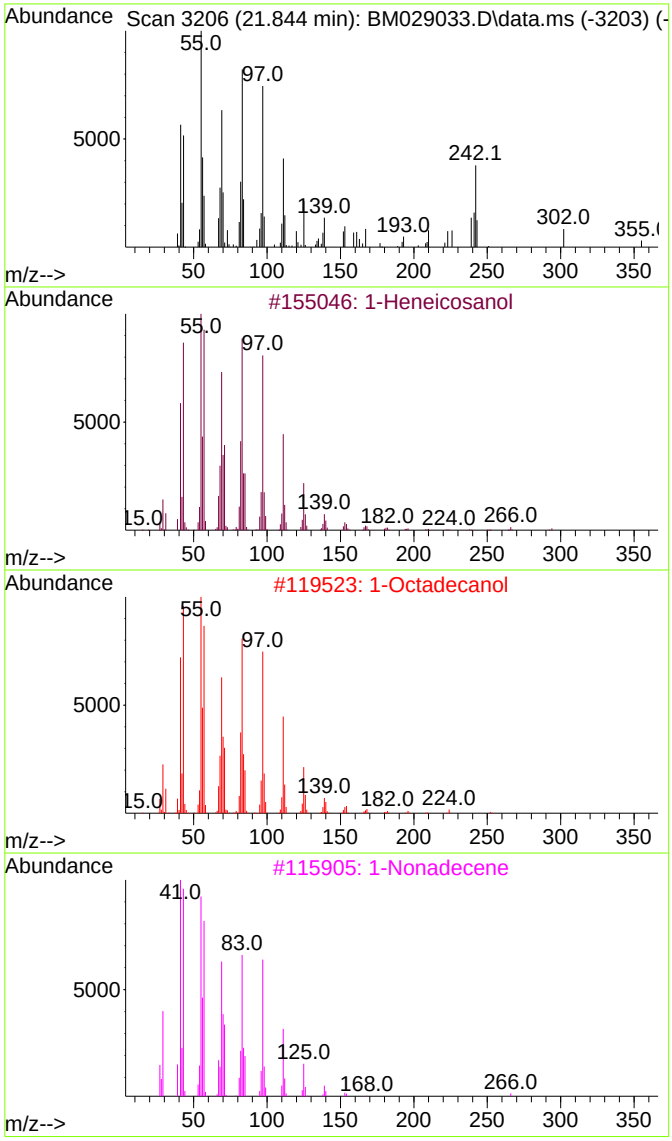
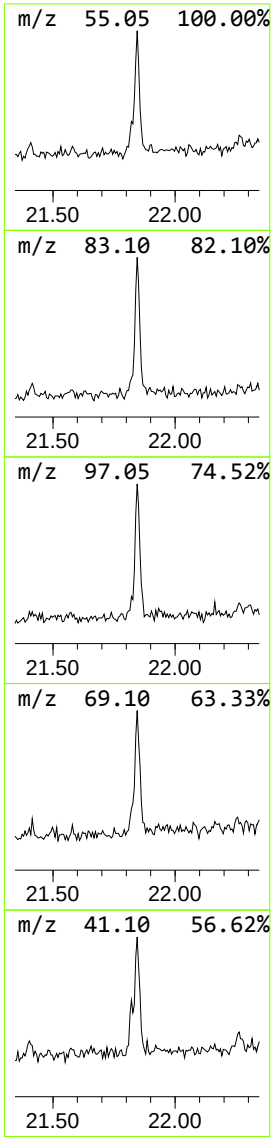
Peak Number 6 1-Heneicosanol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.844	4.82 ng	44578	Chrysene-d12	21.256

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol	312	C21H44O	015594-90-8	87
2	1-Octadecanol	270	C18H38O	000112-92-5	83
3	1-Nonadecene	266	C19H38	018435-45-5	80
4	1-Hexadecene, 16-bromo-	302	C16H31Br	118625-56-2	76
5	Behenic alcohol	326	C22H46O	000661-19-8	74





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Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_M
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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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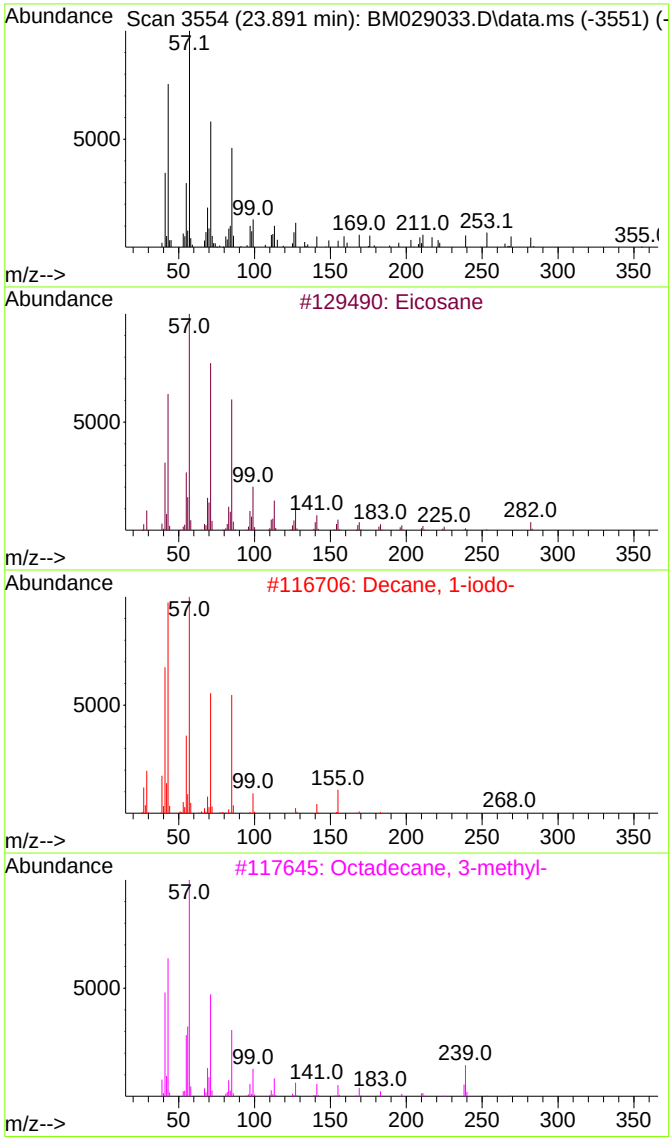
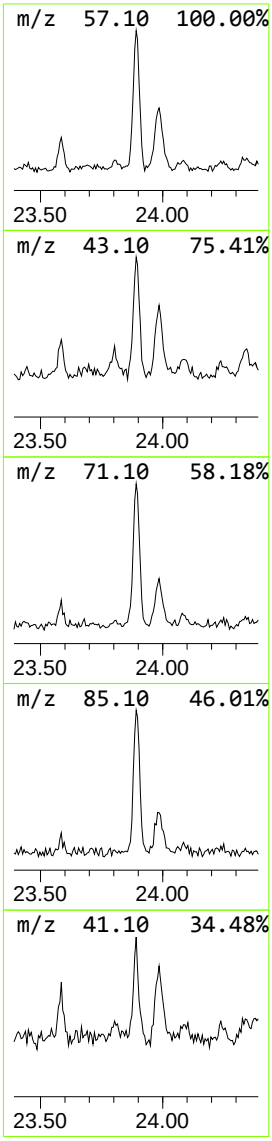
Peak Number 7 Eicosane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.891	5.78 ng	42413	Perylene-d12	23.415

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	96
2	Decane, 1-iodo-	268	C10H21I	002050-77-3	93
3	Octadecane, 3-methyl-	268	C19H40	006561-44-0	87
4	Hexatriacontane	507	C36H74	000630-06-8	86
5	Octacosane	394	C28H58	000630-02-4	80





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM030821\
Data File : BM029033.D
Acq On : 08 Mar 2021 23:46
Operator : CG/JU
Sample : M1591-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : FK-PS-01-070

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

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
unknown14.221	14.221	3.0	ng	14166	3	14.333	95224	20.0
n-Hexadecanoic ...	17.980	10.1	ng	52667	4	17.080	104603	20.0
Pyrene, 1-methyl-	20.003	2.5	ng	22678	5	21.256	184850	20.0
Cyclohexadecane	20.974	9.2	ng	84949	5	21.256	184850	20.0
unknown21.403	21.403	2.0	ng	18554	5	21.256	184850	20.0
1-Heneicosanol	21.844	4.8	ng	44578	5	21.256	184850	20.0
Eicosane	23.891	5.8	ng	42413	6	23.415	146645	20.0