LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM031021\
Data File : BM029069.D
Acq On : 10 Mar 2021 14:41
Operator : CG/JU
Sample : M1576-10
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : IDW-GW805-SO-030421

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: BM029069.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.087	14	17	25	rVB	22028	26046	1.22%	0.309%
2	4.257	212	216	223	rBV	22831	28176	1.32%	0.335%
3	5.240	377	383	391	rBV	144367	203430	9.56%	2.416%
4	6.863	654	659	669	rBV	118827	188239	8.84%	2.235%
5	7.663	790	795	801	rBB	33352	48843	2.30%	0.580%
6	8.839	989	995	1006	rBB	88825	142736	6.71%	1.695%
7	10.457	1264	1270	1277	rBV	39306	63823	3.00%	0.758%
8	12.945	1688	1693	1702	rBV	196887	287363	13.50%	3.413%
9	14.333	1918	1929	1936	rBV	58587	104875	4.93%	1.245%
10	15.292	2045	2092	2094	rBV2	107108	766931	36.04%	9.108%
11	15.839	2179	2185	2199	rVB	200218	306439	14.40%	3.639%
12	17.086	2392	2397	2402	rVB	68205	92308	4.34%	1.096%
13	17.598	2471	2484	2499	rVB3	20107	87190	4.10%	1.035%
14	18.004	2537	2553	2576	rVB	703044	1435796	67.46%	17.051%
15	18.521	2637	2641	2646	rVB2	17768	21846	1.03%	0.259%
16	19.062	2728	2733	2737	rBV	23353	34079	1.60%	0.405%
17	19.121	2738	2743	2745	rVV2	56098	84162	3.95%	0.999%
18	19.151	2745	2748	2757	rVV2	89110	223330	10.49%	2.652%
19	19.286	2759	2771	2795	rVB	1108073	2128227	100.00%	25.274%
20	19.709	2838	2843	2847	rBV	466114	649145	30.50%	7.709%
21	20.127	2908	2914	2919	rBV2	41760	91976	4.32%	1.092%
22	20.186	2919	2924	2933	rVB	89244	175399	8.24%	2.083%
23	20.986	3053	3060	3068	rBV	146917	269495	12.66%	3.200%
24	21.256	3102	3106	3111	rBV	85954	109510	5.15%	1.300%
25	21.662	3169	3175	3183	rBV	140353	240254	11.29%	2.853%
26	22.350	3286	3292	3300	rVB	112463	223764	10.51%	2.657%
27	23.121	3416	3423	3430	rBV	83140	172247	8.09%	2.046%
28	23.421	3469	3474	3481	rVB2	59306	109244	5.13%	1.297%
29	23.991	3565	3571	3580	rVB3	42753	105890	4.98%	1.257%

Sum of corrected areas: 8420763

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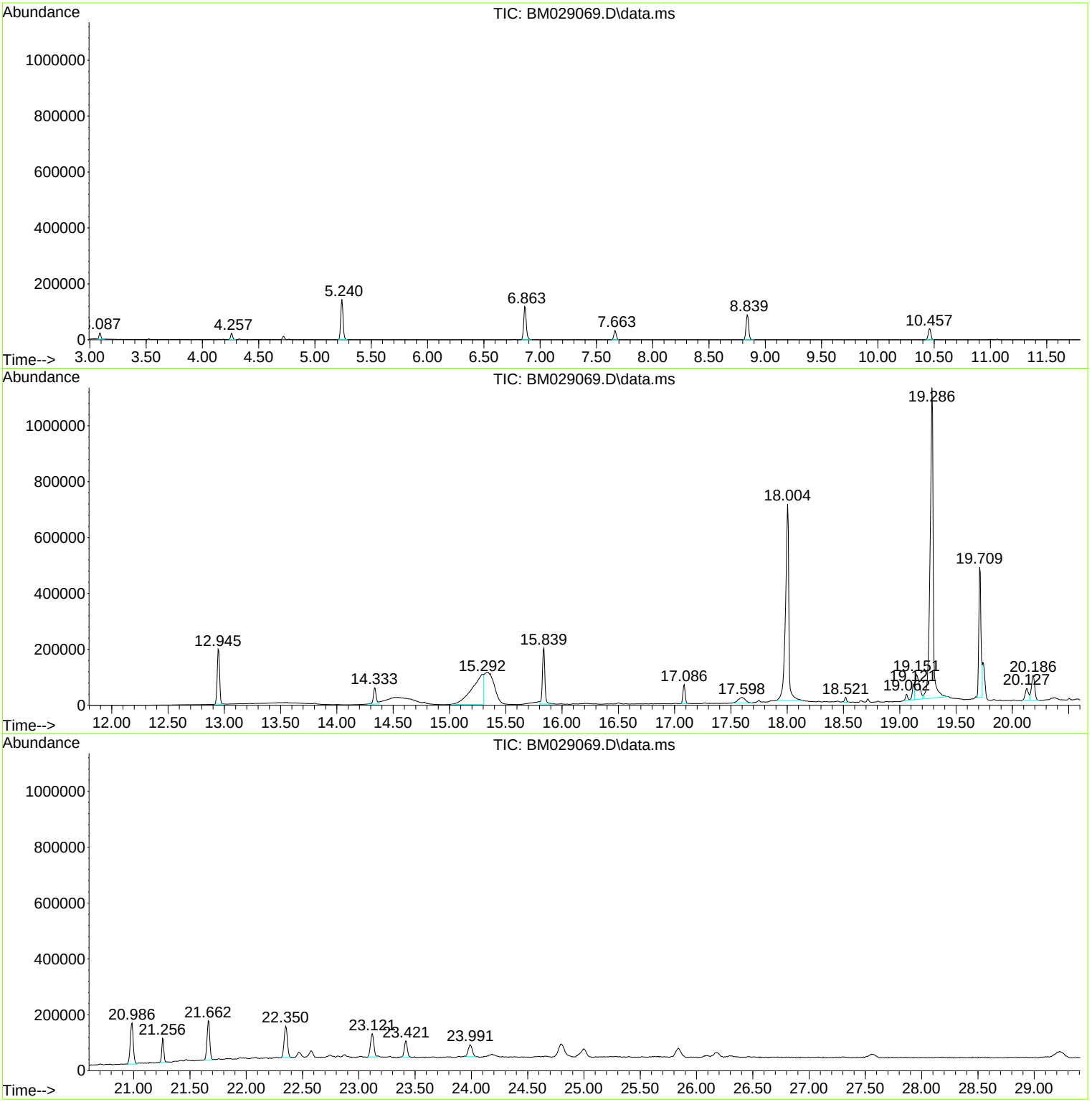
ClientSampleId :
IDW-GW805-SO-030421

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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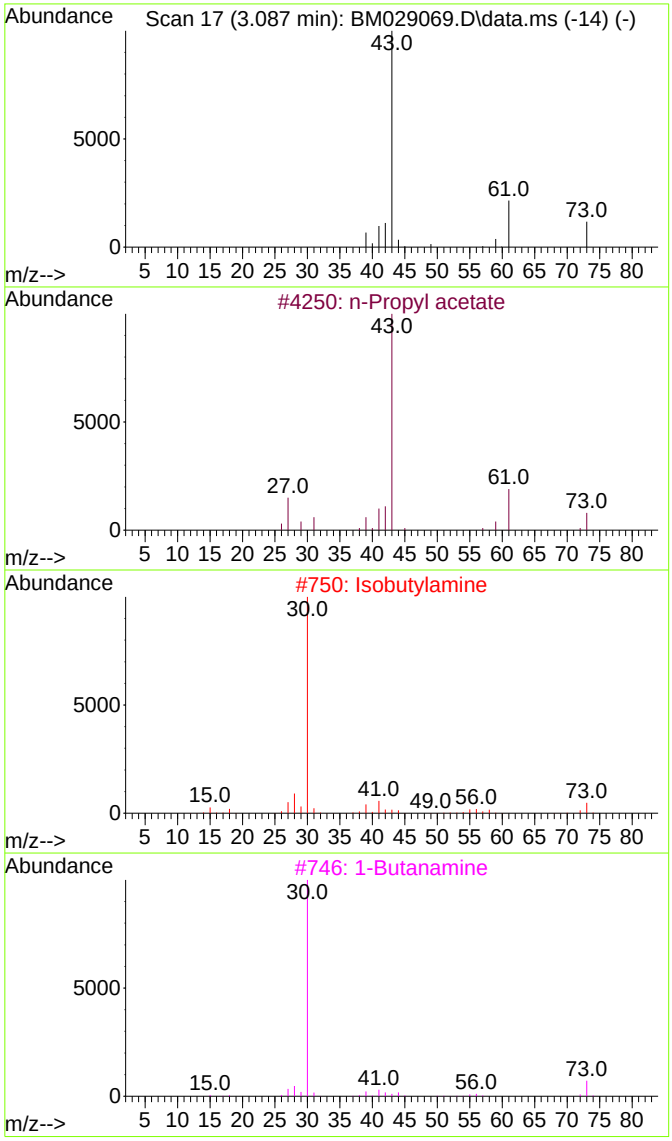
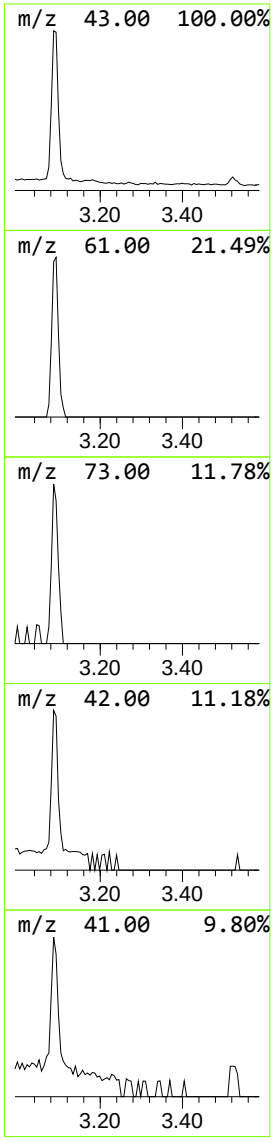
Peak Number 1 n-Propyl acetate Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.087	10.67 ng	26046	1,4-Dichlorobenzene-d4	7.669

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Propyl acetate	102	C5H10O2	000109-60-4	64
2	Isobutylamine	73	C4H11N	000078-81-9	4
3	1-Butanamine	73	C4H11N	000109-73-9	4
4	Hydrogen azide	43	HN3	007782-79-8	4
5	1,4-Butanediol, diacetate	174	C8H14O4	000628-67-1	4





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Instrument : BNA_M
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM022321.M
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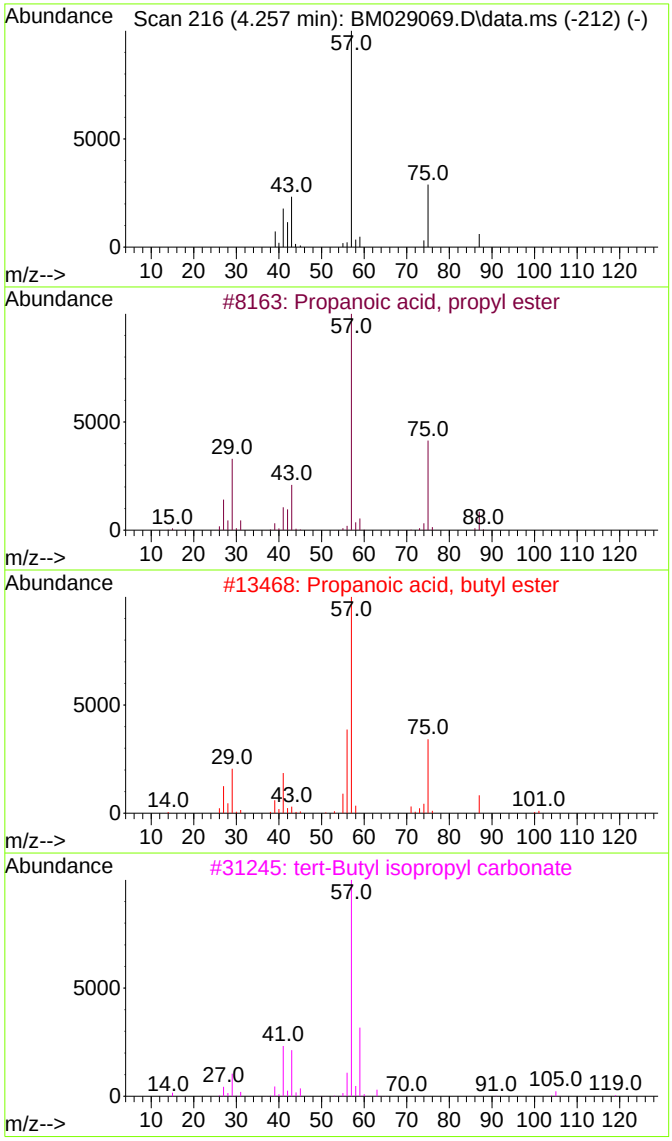
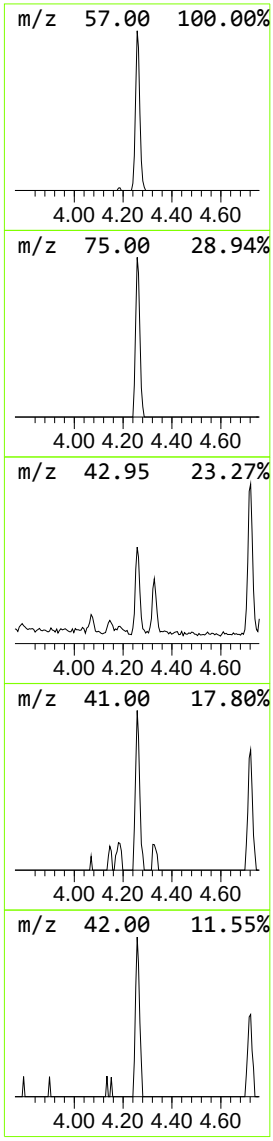
Peak Number 2 Propanoic acid, propyl ester Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.257	11.54 ng	28176	1,4-Dichlorobenzene-d4	7.669

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	78
2	Propanoic acid, butyl ester	130	C7H14O2	000590-01-2	36
3	tert-Butyl isopropyl carbonate	160	C8H16O3	030221-21-7	9
4	Azetidine	57	C3H7N	000503-29-7	7
5	S-(-)-2-Methylbutylamine	87	C5H13N	020626-52-2	5





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ClientSampleId :
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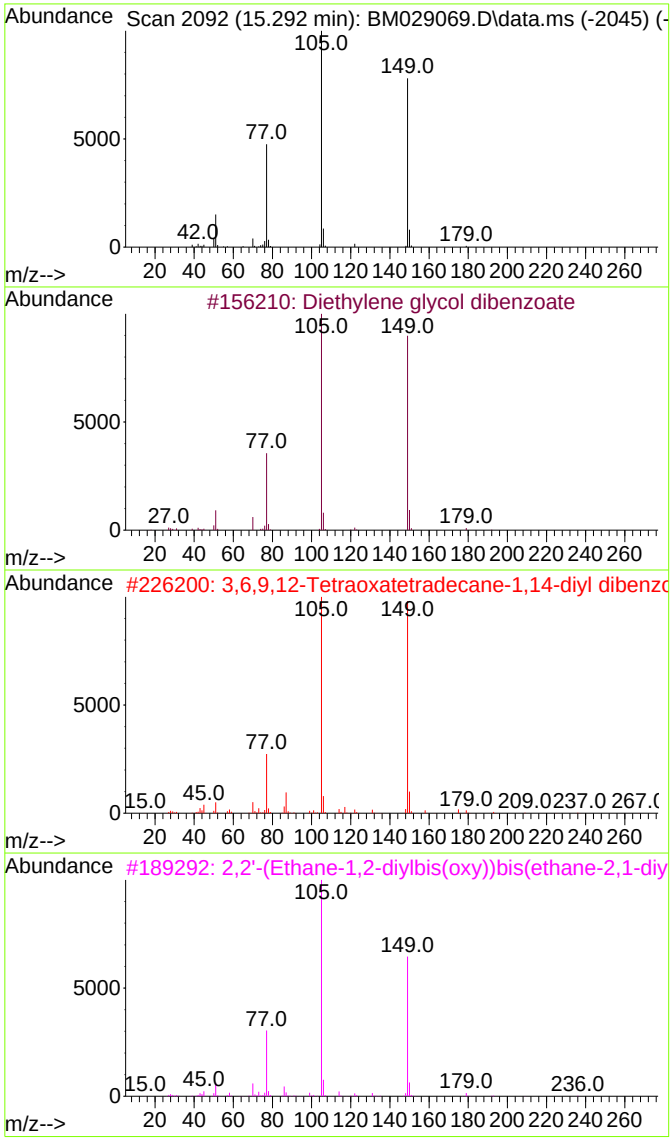
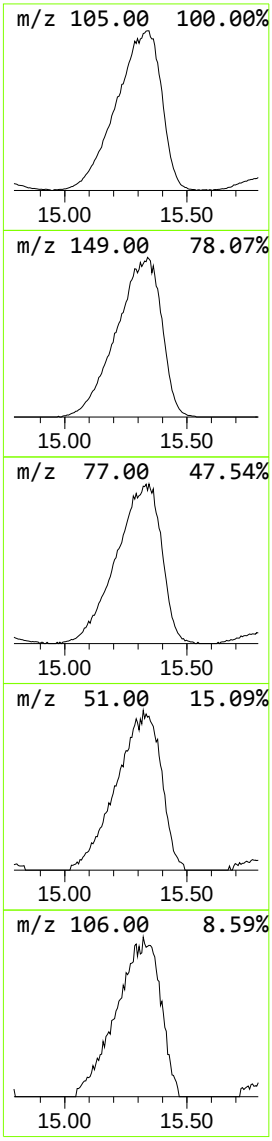
Peak Number 3 Diethylene glycol dibenzoate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.292	146.26 ng	766931	Acenaphthene-d10	14.333

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Diethylene glycol dibenzoate	314	C18H18O5	000120-55-8	83
2	3,6,9,12-Tetraoxatetradecane-1,1...	446	C24H30O8	1000366-97-0	72
3	2,2'-(Ethane-1,2-diylbis(oxy))bi...	358	C20H22O6	1000366-99-4	64
4	Cyclobutyl phenyl ketone	160	C11H12O	005407-98-7	35
5	Benzeneacetic acid, .alpha.-oxo-...	164	C9H8O3	015206-55-0	35





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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM022321.M
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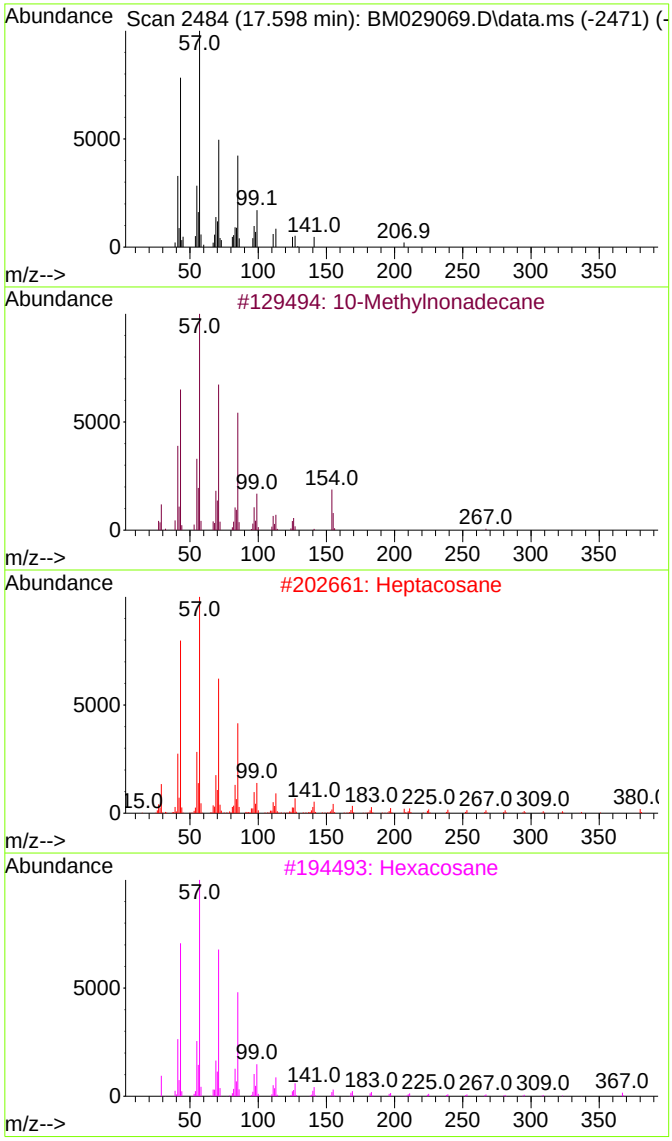
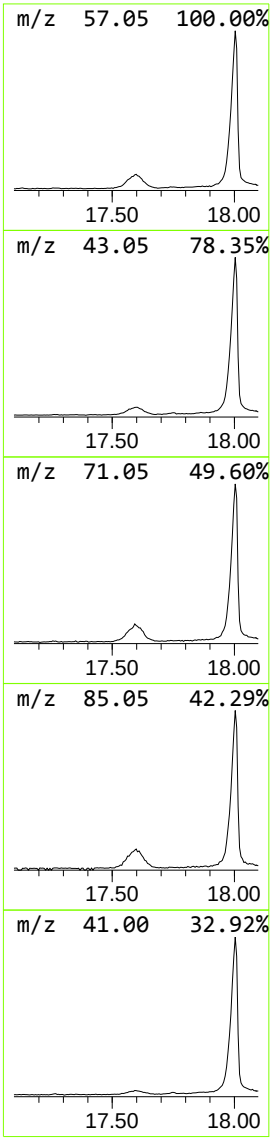
Peak Number 4 10-Methylnonadecane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.598	18.89 ng	87190	Phenanthrene-d10	17.086

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	10-Methylnonadecane	282	C20H42	056862-62-5	91
2	Heptacosane	380	C27H56	000593-49-7	91
3	Hexacosane	366	C26H54	000630-01-3	91
4	Heneicosane	296	C21H44	000629-94-7	91
5	Nonadecane	268	C19H40	000629-92-5	90





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Instrument : BNA_M
ClientSampleId : IDW-GW805-SO-030421

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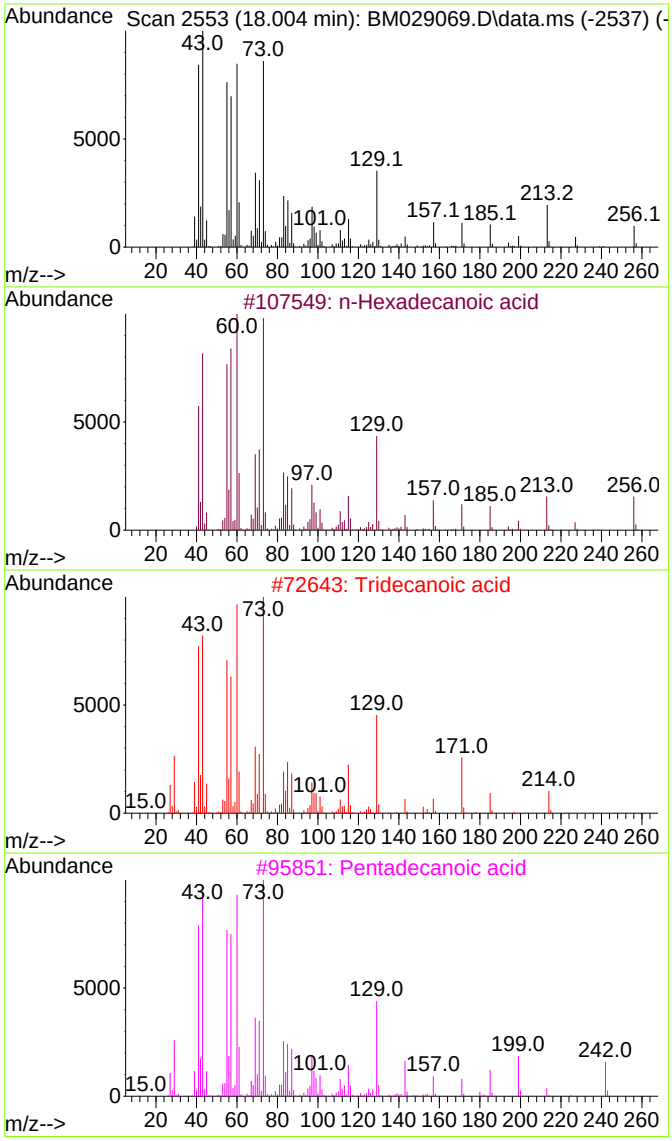
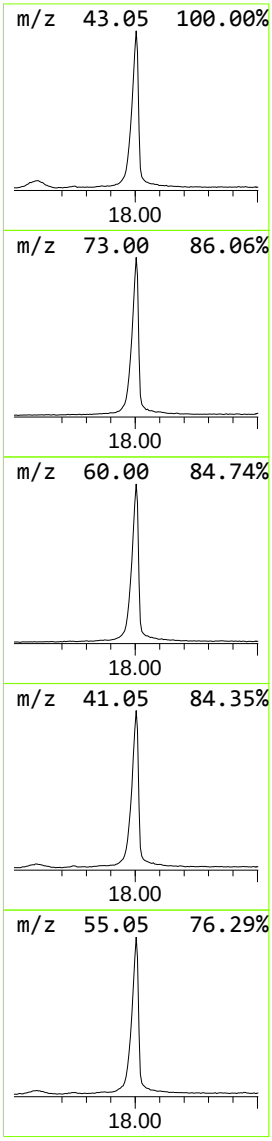
Peak Number 5 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.003	311.09 ng	1435800	Phenanthrene-d10	17.086

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tridecanoic acid	214	C13H26O2	000638-53-9	95
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	81
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	72
5	n-Decanoic acid	172	C10H20O2	000334-48-5	60





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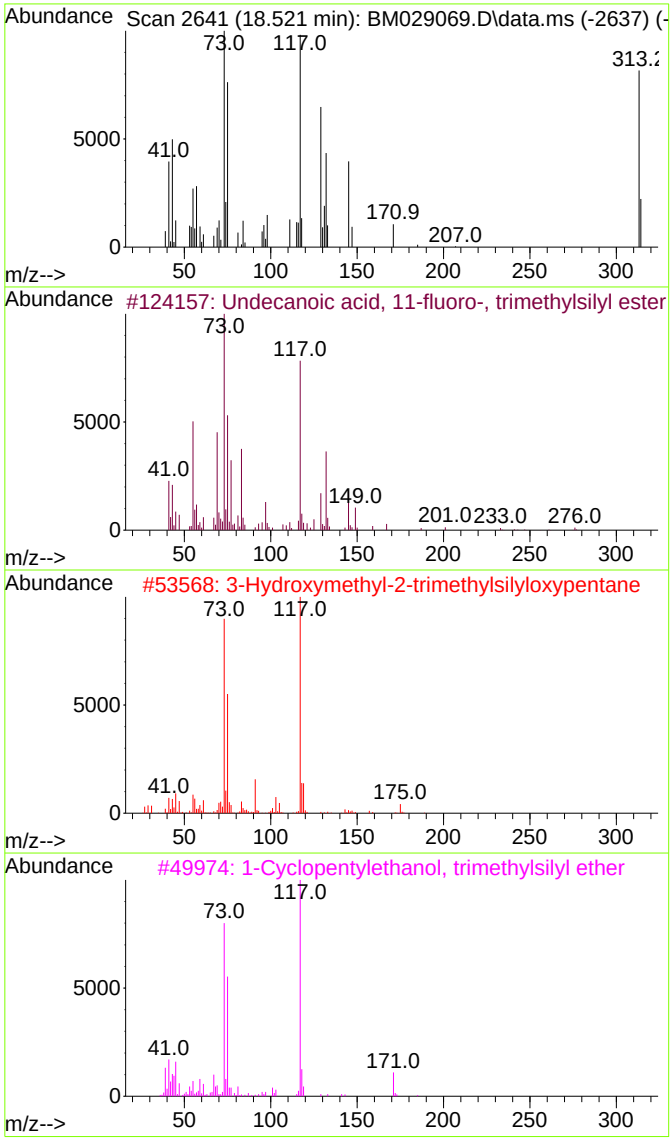
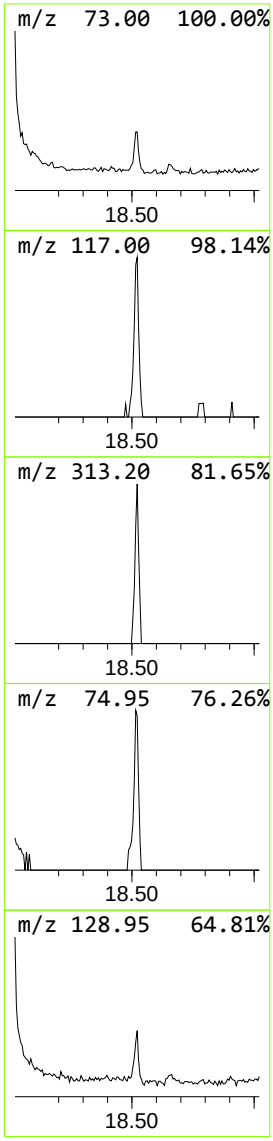
Peak Number 6 unknown18.52 Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.521	4.73 ng	21846	Phenanthrene-d10	17.086

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Undecanoic acid, 11-fluoro-, tri...	276	C14H29FO2Si	026305-97-5	43
2	3-Hydroxymethyl-2-trimethylsilyl...	190	C9H22O2Si	1000189-44-6	27
3	1-Cyclopentylethanol, trimethyls...	186	C10H22OSi	959233-05-7	27
4	4,4-Dimethyl-2-pentanol, trimeth...	188	C10H24OSi	1000364-14-6	27
5	Silane, trimethyl[(1-methylpenty...	174	C9H22OSi	017888-63-0	27





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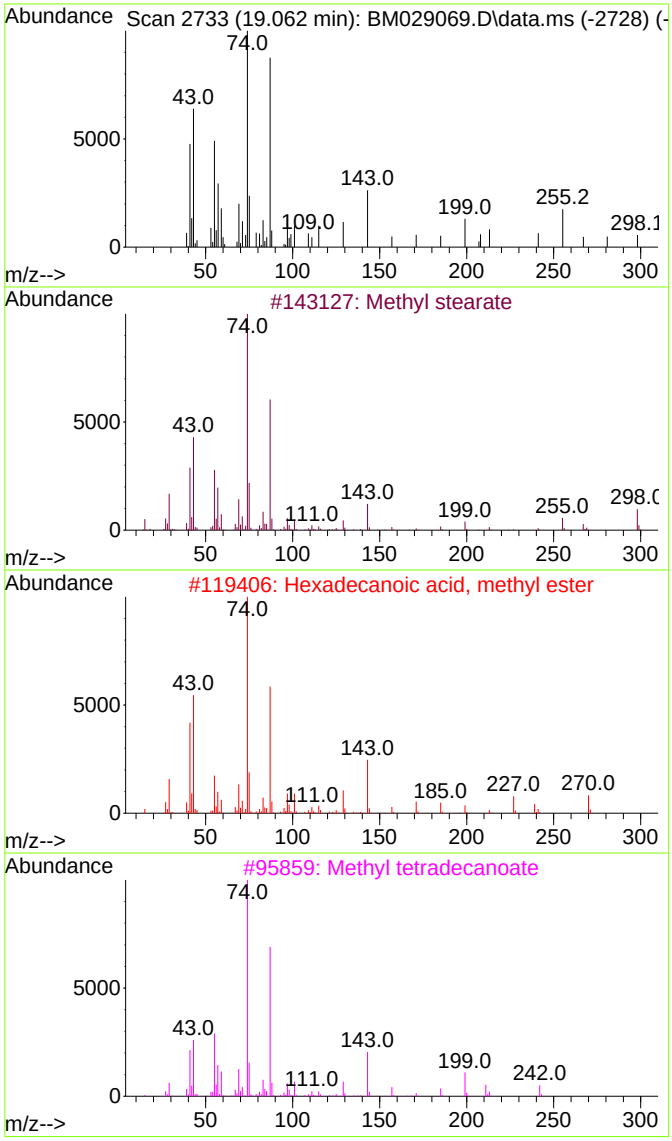
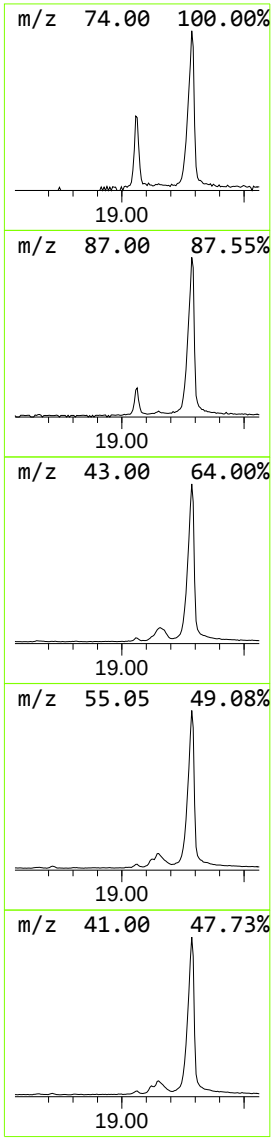
Peak Number 7 Methyl stearate Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.062	7.38 ng	34079	Phenanthrene-d10	17.086

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Methyl stearate	298	C19H38O2	000112-61-8	95
2	Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	80
3	Methyl tetradecanoate	242	C15H30O2	000124-10-7	78
4	Dodecanoic acid, 10-methyl-, met...	228	C14H28O2	005129-65-7	78
5	Tridecanoic acid, 12-methyl-, me...	242	C15H30O2	005129-58-8	72





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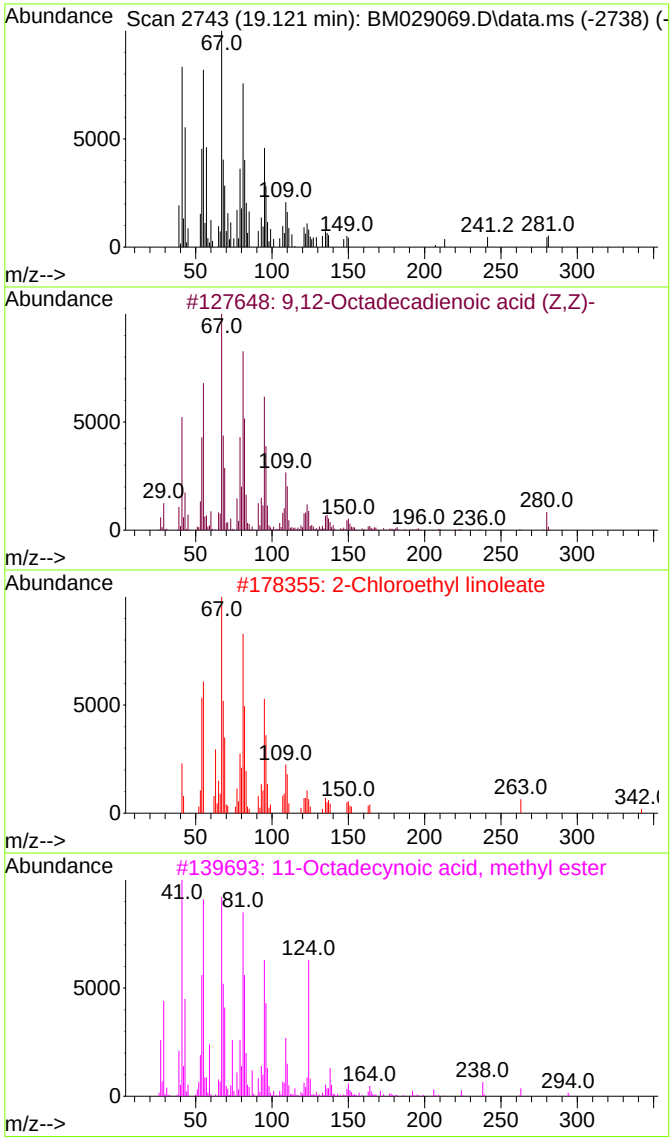
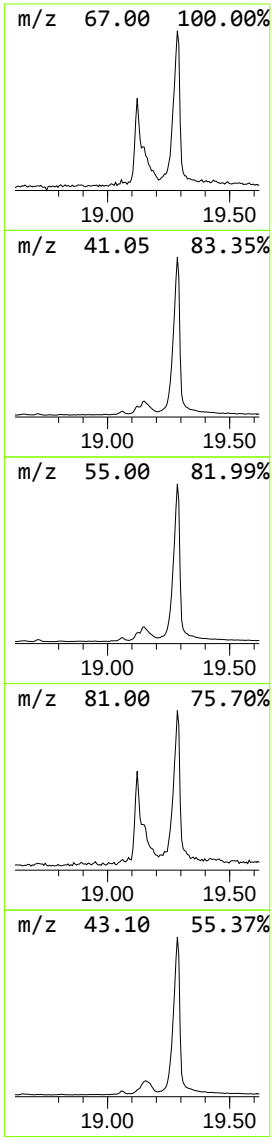
Peak Number 8 9,12-Octadecadienoic acid (... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.121	18.23 ng	84162	Phenanthrene-d10	17.086

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9,12-Octadecadienoic acid (Z,Z)-	280	C18H32O2	000060-33-3	98
2	2-Chloroethyl linoleate	342	C20H35ClO2	025525-76-2	91
3	11-Octadecynoic acid, methyl ester	294	C19H34O2	026543-37-3	91
4	Bicyclo[2.2.2]octane, 2-methyl-	124	C9H16	000766-53-0	91
5	1-Tetradecyne	194	C14H26	000765-10-6	86





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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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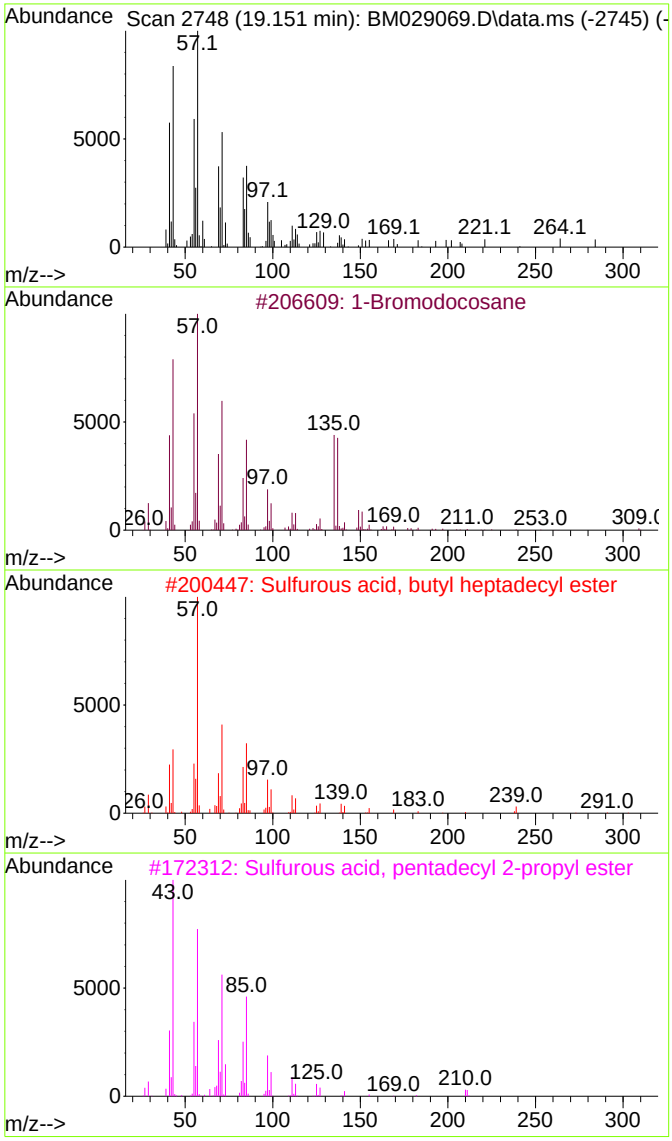
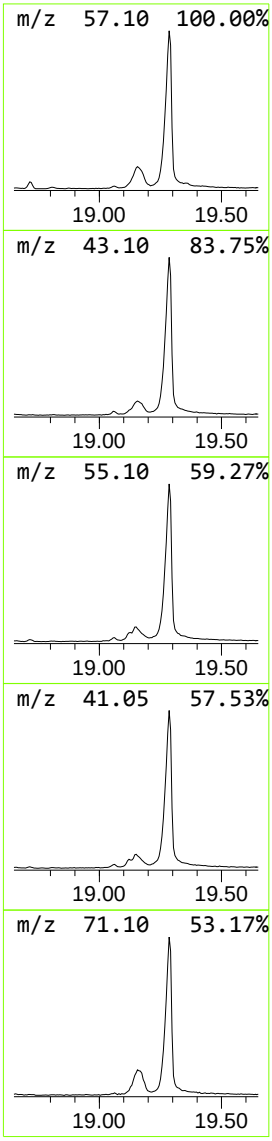
Peak Number 9 1-Bromodocosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.151	48.39 ng	223330	Phenanthrene-d10	17.086

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Bromodocosane	388	C22H45Br	006938-66-5	72
2	Sulfurous acid, butyl heptadecyl...	376	C21H44O3S	1000309-18-4	72
3	Sulfurous acid, pentadecyl 2-pro...	334	C18H38O3S	1000309-12-6	72
4	Sulfurous acid, butyl octadecyl ...	390	C22H46O3S	1000309-18-5	72
5	Sulfurous acid, octadecyl 2-prop...	376	C21H44O3S	1000309-12-7	72





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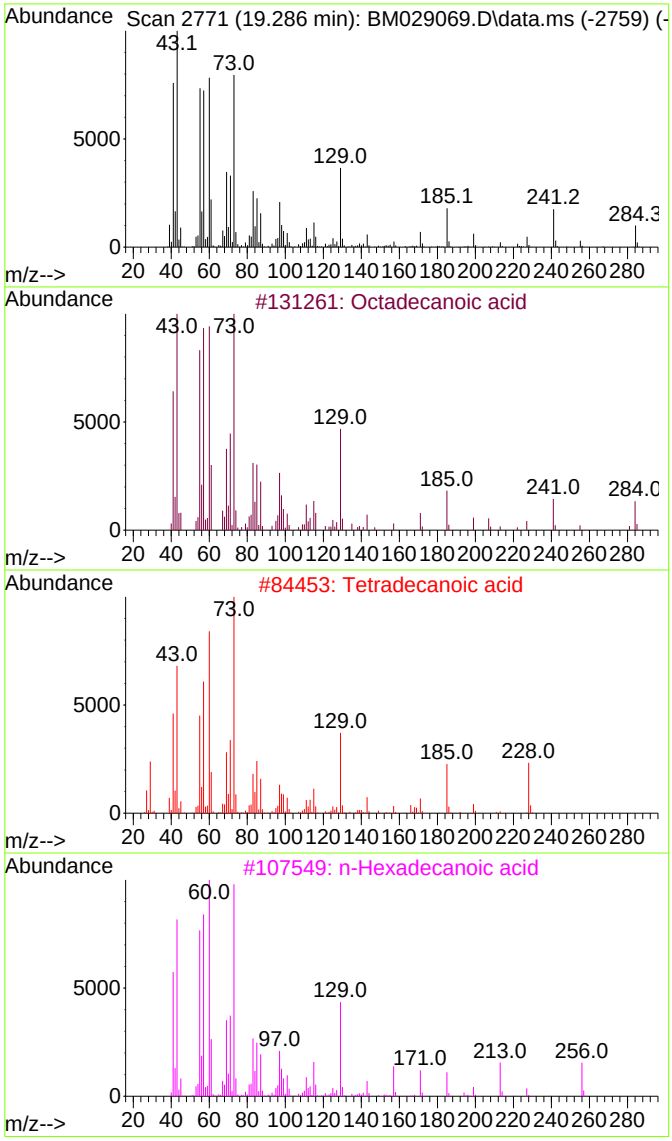
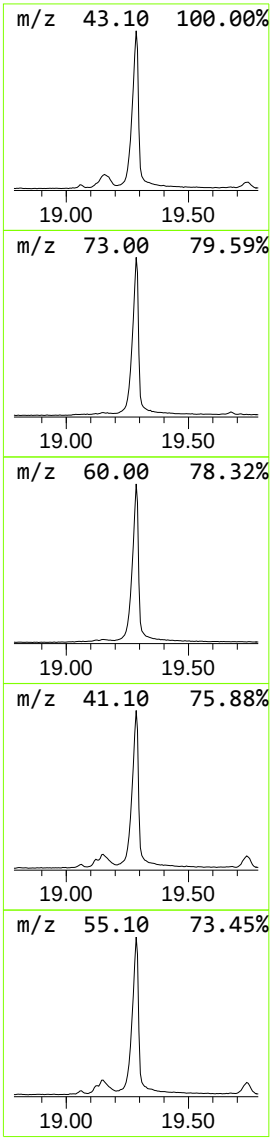
Peak Number 10 Octadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.286	388.68 ng	2128230	Chrysene-d12	21.256

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	81
3	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	72
4	Undecanoic acid	186	C11H22O2	000112-37-8	70
5	Pentadecanoic acid	242	C15H30O2	001002-84-2	60





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Acq On : 10 Mar 2021 14:41
Operator : CG/JU
Sample : M1576-10
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
IDW-GW805-SO-030421

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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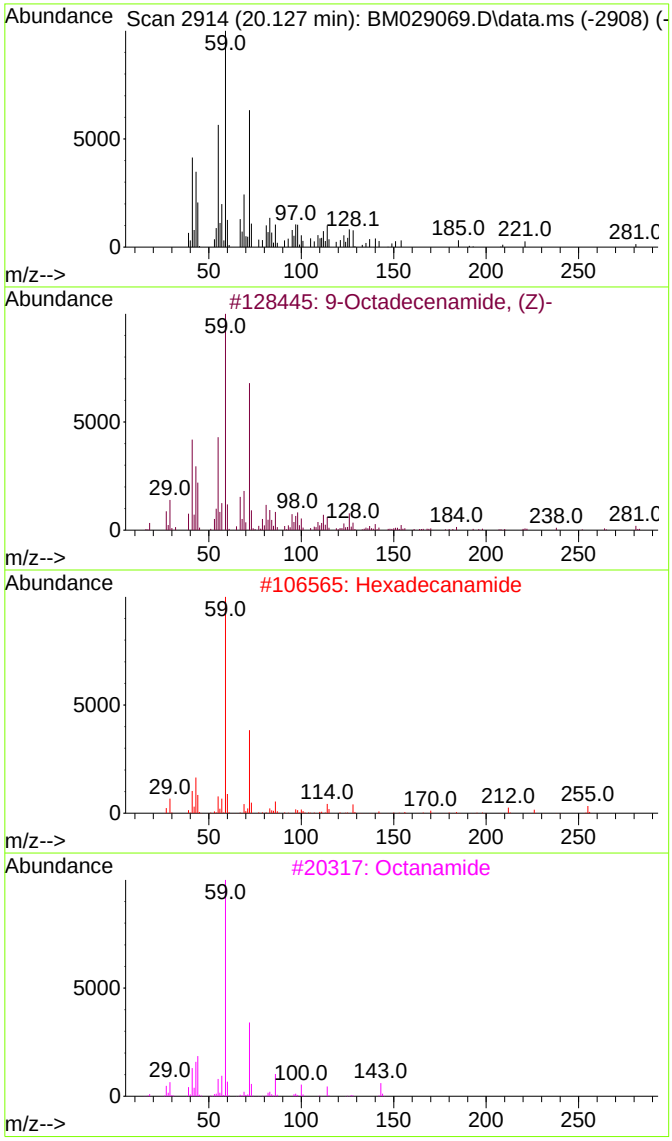
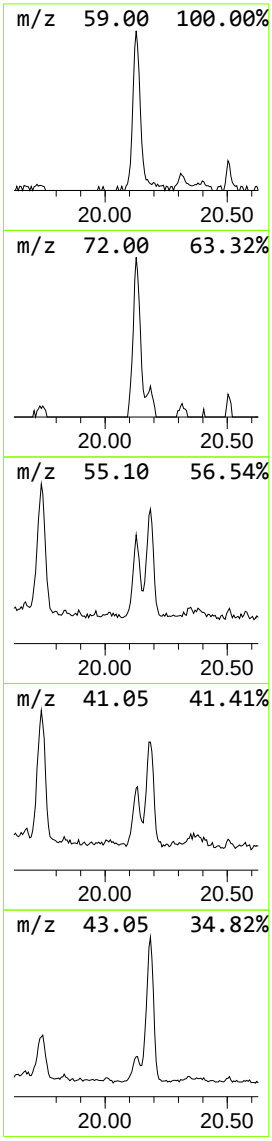
Peak Number 11 9-Octadecenamide, (Z)- Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.127	16.80 ng	91976	Chrysene-d12	21.256

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	96
2	Hexadecanamide	255	C16H33NO	000629-54-9	64
3	Octanamide	143	C8H17NO	000629-01-6	59
4	Dodecanamide	199	C12H25NO	001120-16-7	59
5	Benzeneethanamine, 2-fluoro-.bet...	229	C11H16FNO3	061338-98-5	59





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Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
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ClientSampleId :
IDW-GW805-SO-030421

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

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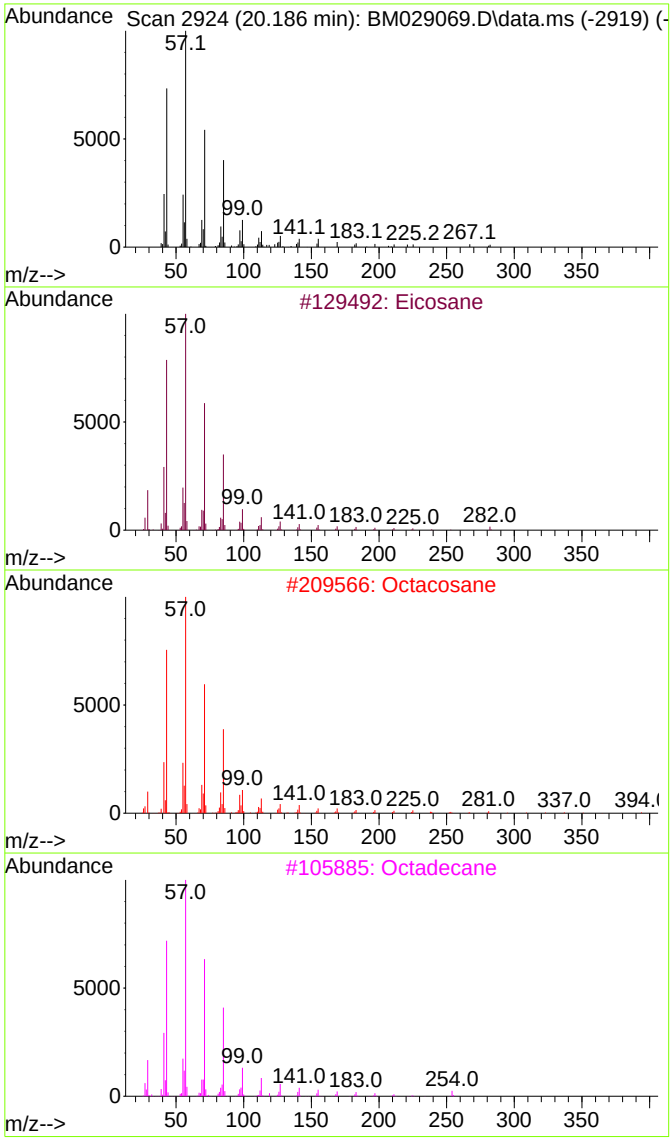
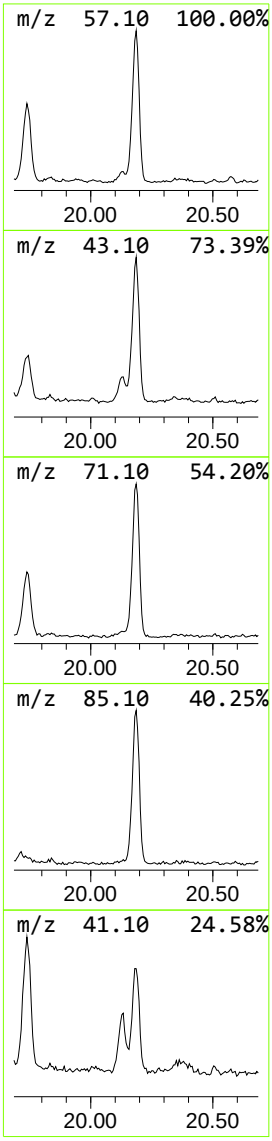
Peak Number 12 Eicosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.186	32.03 ng	175399	Chrysene-d12	21.256

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	96
2	Octacosane	394	C28H58	000630-02-4	91
3	Octadecane	254	C18H38	000593-45-3	91
4	Heptacosane	380	C27H56	000593-49-7	91
5	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91





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ALS Vial : 5 Sample Multiplier: 1

Instrument :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
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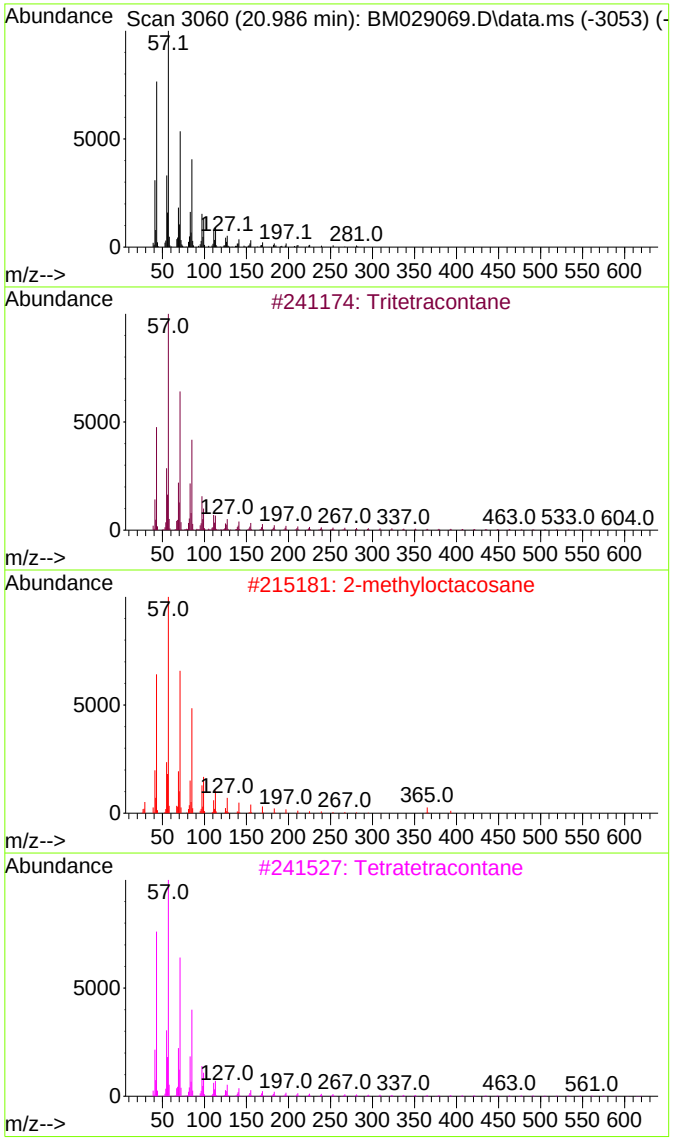
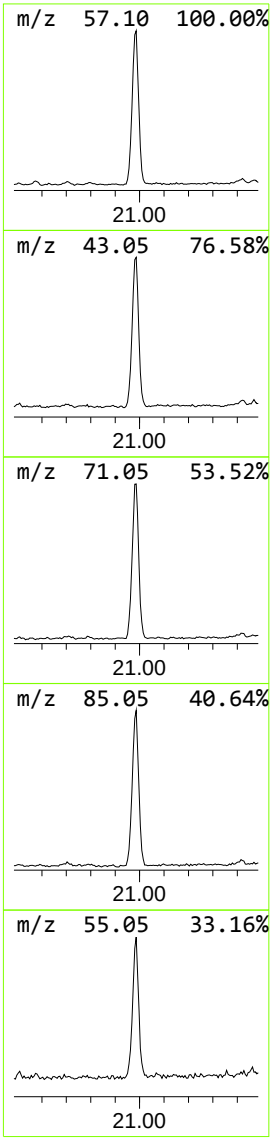
Peak Number 13 Tritetracontane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.986	49.22 ng	269495	Chrysene-d12	21.256

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tritetracontane	605	C43H88	007098-21-7	91
2	2-methyloctacosane	408	C29H60	1000376-72-8	91
3	Tetratetracontane	619	C44H90	007098-22-8	91
4	10-Methylnonadecane	282	C20H42	056862-62-5	91
5	2-methyltetracosane	352	C25H52	1000376-72-6	91





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Misc :
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Instrument :
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ClientSampleId :
IDW-GW805-SO-030421

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM022321.M
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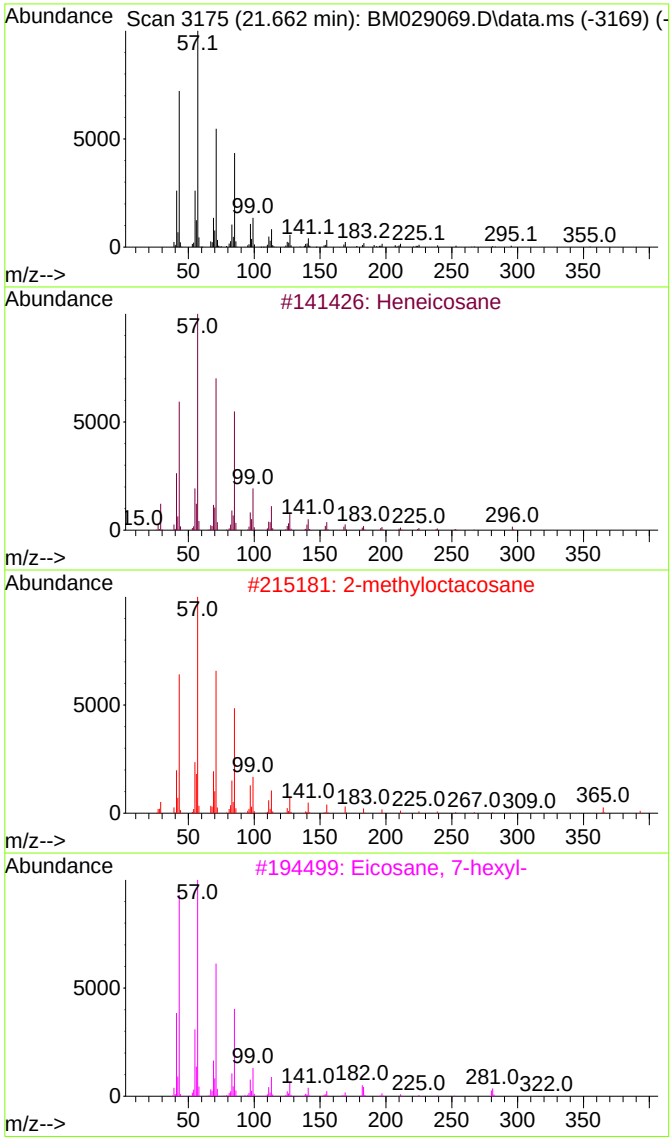
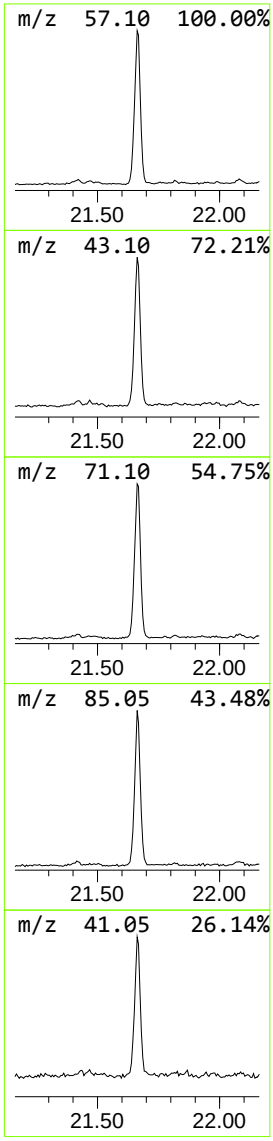
Peak Number 14 Heneicosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.662	43.88 ng	240254	Chrysene-d12	21.256

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	91
2	2-methyloctacosane	408	C29H60	1000376-72-8	91
3	Eicosane, 7-hexyl-	366	C26H54	055333-99-8	91
4	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
5	Tetracosane	338	C24H50	000646-31-1	91





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Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : IDW-GW805-SO-030421

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

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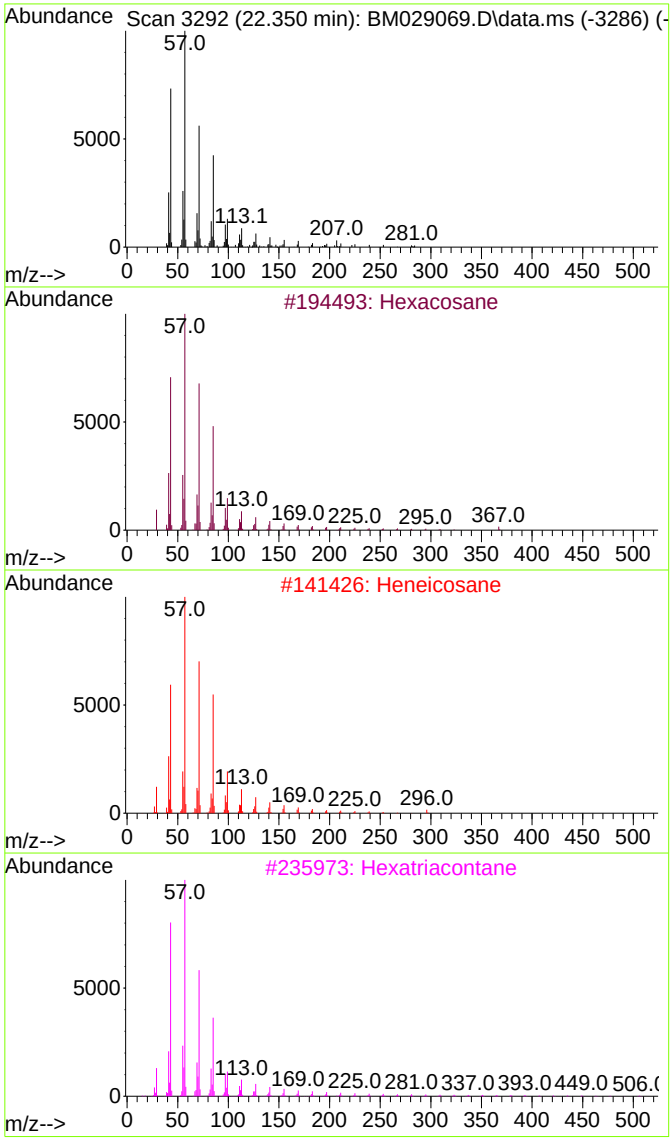
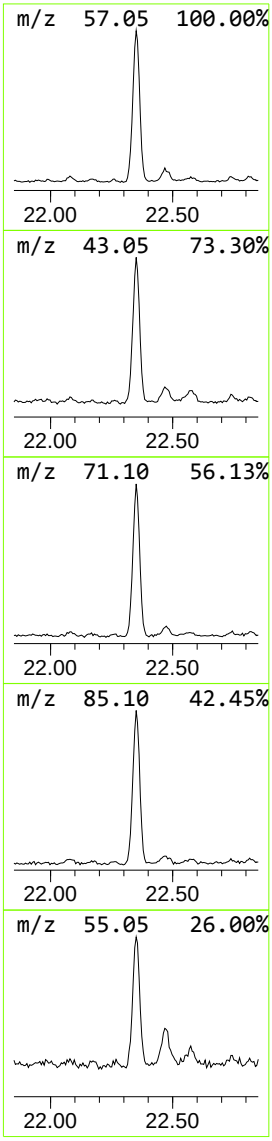
Peak Number 15 Hexacosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.350	40.97 ng	223764	Perylene-d12	23.421

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosane	366	C26H54	000630-01-3	94
2	Heneicosane	296	C21H44	000629-94-7	91
3	Hexatriacontane	507	C36H74	000630-06-8	91
4	Pentacosane	352	C25H52	000629-99-2	91
5	2-methyloctacosane	408	C29H60	1000376-72-8	91





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ALS Vial : 5 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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TIC Library : C:\DATABASE\NIST11.L
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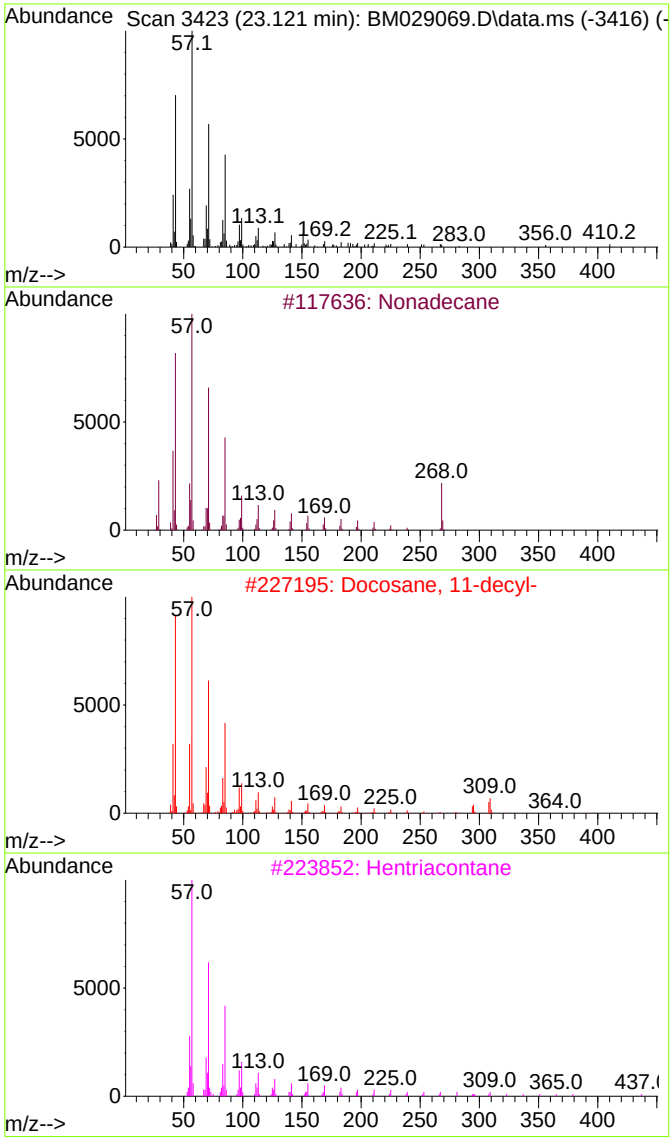
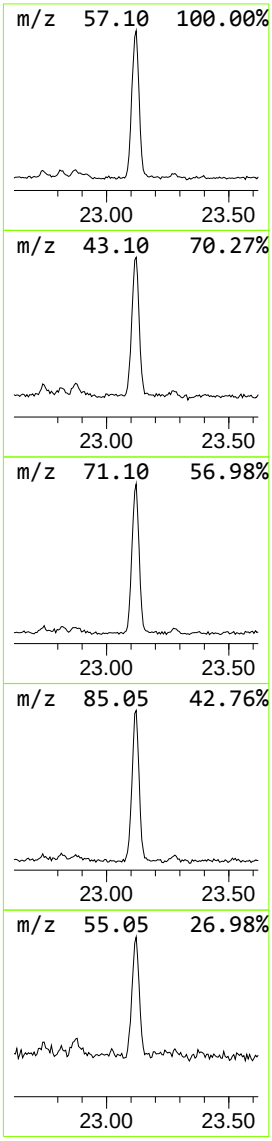
Peak Number 16 Nonadecane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.121	31.53 ng	172247	Perylene-d12	23.421

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonadecane	268	C19H40	000629-92-5	96
2	Docosane, 11-decyl-	451	C32H66	055401-55-3	90
3	Hentriacontane	437	C31H64	000630-04-6	90
4	Triacontane	422	C30H62	000638-68-6	90
5	Octacosane	394	C28H58	000630-02-4	90





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Operator : CG/JU
Sample : M1576-10
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
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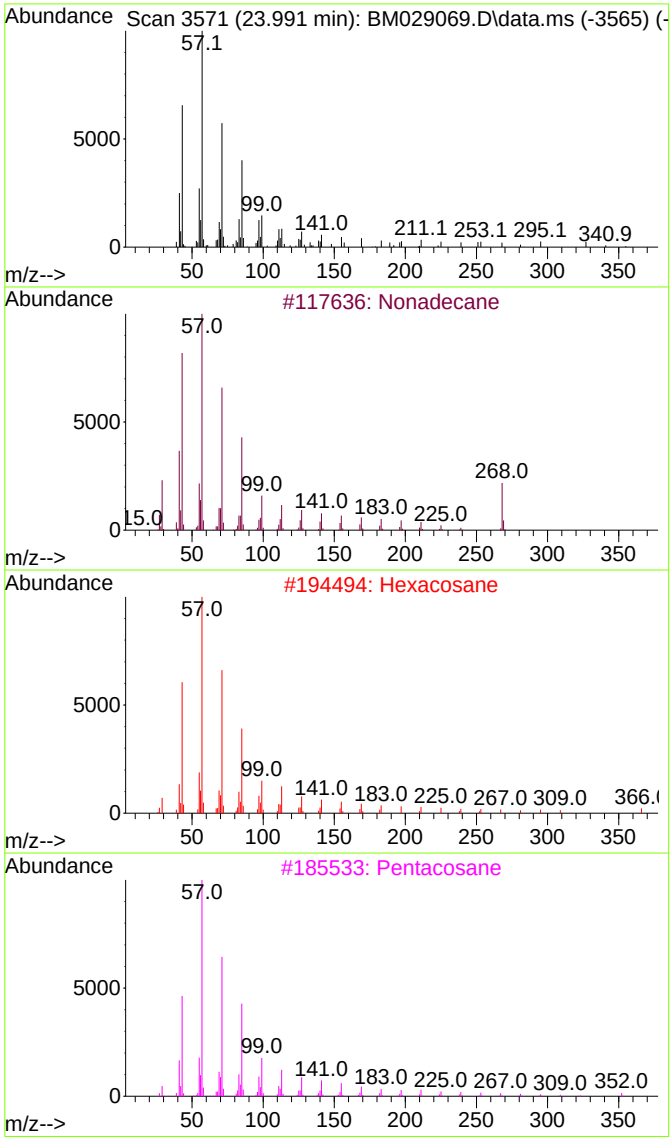
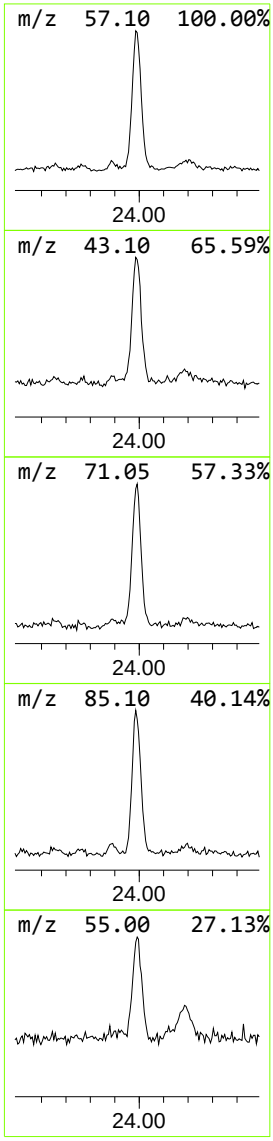
Peak Number 17 Pentacosane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.991	19.39 ng	105890	Perylene-d12	23.421

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonadecane	268	C19H40	000629-92-5	95
2	Hexacosane	366	C26H54	000630-01-3	91
3	Pentacosane	352	C25H52	000629-99-2	90
4	Hentriacontane	437	C31H64	000630-04-6	90
5	Tetracosane, 11-decyl-	479	C34H70	055429-84-0	90





Tentatively Identified Compound (LSC) summary

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Data File : BM029069.D
Acq On : 10 Mar 2021 14:41
Operator : CG/JU
Sample : M1576-10
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : IDW-GW805-SO-030421

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
n-Propyl acetate	3.087	10.7	ng	26046	1	7.669	48843	20.0
Propanoic acid,...	4.257	11.5	ng	28176	1	7.669	48843	20.0
Diethylene glyc...	15.292	146.3	ng	766931	3	14.333	104875	20.0
10-Methylnonade...	17.598	18.9	ng	87190	4	17.086	92308	20.0
n-Hexadecanoic ...	18.003	311.1	ng	1435800	4	17.086	92308	20.0
unknown18.52	18.521	4.7	ng	21846	4	17.086	92308	20.0
Methyl stearate	19.062	7.4	ng	34079	4	17.086	92308	20.0
9,12-Octadecadi...	19.121	18.2	ng	84162	4	17.086	92308	20.0
1-Bromodocosane	19.151	48.4	ng	223330	4	17.086	92308	20.0
Octadecanoic acid	19.286	388.7	ng	2128230	5	21.256	109510	20.0
9-Octadecenamid...	20.127	16.8	ng	91976	5	21.256	109510	20.0
Eicosane	20.186	32.0	ng	175399	5	21.256	109510	20.0
Tritetracontane	20.986	49.2	ng	269495	5	21.256	109510	20.0
Heneicosane	21.662	43.9	ng	240254	5	21.256	109510	20.0
Hexacosane	22.350	41.0	ng	223764	6	23.421	109244	20.0
Nonadecane	23.121	31.5	ng	172247	6	23.421	109244	20.0
Pentacosane	23.991	19.4	ng	105890	6	23.421	109244	20.0