LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM030821\
Data File : BM029030.D
Acq On : 08 Mar 2021 21:57
Operator : CG/JU
Sample : M1582-03
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : RO-363

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: BM029030.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.363	61	64	79	rBV	41491	56891	19.56%	2.111%
2	5.246	379	384	395	rBB	203321	285233	98.07%	10.583%
3	6.869	654	660	674	rBV	188659	290849	100.00%	10.792%
4	7.669	791	796	802	rBB	43209	62611	21.53%	2.323%
5	8.845	989	996	1007	rBB	117202	183680	63.15%	6.815%
6	10.463	1264	1271	1279	rBB	52826	82688	28.43%	3.068%
7	12.951	1688	1694	1701	rBB	186551	259895	89.36%	9.643%
8	13.286	1746	1751	1763	rBV	6216	13710	4.71%	0.509%
9	13.804	1835	1839	1843	rBB	3573	4308	1.48%	0.160%
10	14.222	1901	1910	1916	rBV4	4287	10313	3.55%	0.383%
11	14.339	1924	1930	1936	rVB	72166	102400	35.21%	3.800%
12	15.833	2179	2184	2192	rBV	202695	267236	91.88%	9.916%
13	16.757	2336	2341	2348	rBV3	2231	4885	1.68%	0.181%
14	17.086	2390	2397	2402	rBV	83784	113766	39.12%	4.221%
15	17.127	2402	2404	2408	rVB	2771	3022	1.04%	0.112%
16	17.980	2541	2549	2558	rBV	38975	50109	17.23%	1.859%
17	18.721	2671	2675	2677	rBV	3412	4530	1.56%	0.168%
18	18.751	2677	2680	2687	rVB	9184	13546	4.66%	0.503%
19	19.139	2742	2746	2752	rVB	10532	13081	4.50%	0.485%
20	19.262	2763	2767	2775	rBV2	12589	15914	5.47%	0.590%
21	19.504	2801	2808	2813	rVB	8423	11023	3.79%	0.409%
22	19.709	2838	2843	2848	rBV	239532	272854	93.81%	10.124%
23	19.998	2888	2892	2899	rVB8	2090	3955	1.36%	0.147%
24	20.321	2943	2947	2958	rBV	27742	42371	14.57%	1.572%
25	20.968	3053	3057	3064	rBV	59992	80979	27.84%	3.005%
26	21.256	3101	3106	3110	rBV	118223	140906	48.45%	5.228%
27	21.292	3110	3112	3116	rVB	5386	5205	1.79%	0.193%
28	21.592	3159	3163	3172	rBV	47931	73043	25.11%	2.710%
29	21.845	3204	3206	3212	rVB5	8425	11464	3.94%	0.425%
30	22.892	3380	3384	3394	rBV	21796	43778	15.05%	1.624%
31	23.415	3467	3473	3480	rBV	79425	138358	47.57%	5.134%
32	23.986	3565	3570	3578	rVB6	14200	32472	11.16%	1.205%

Sum of corrected areas: 2695075

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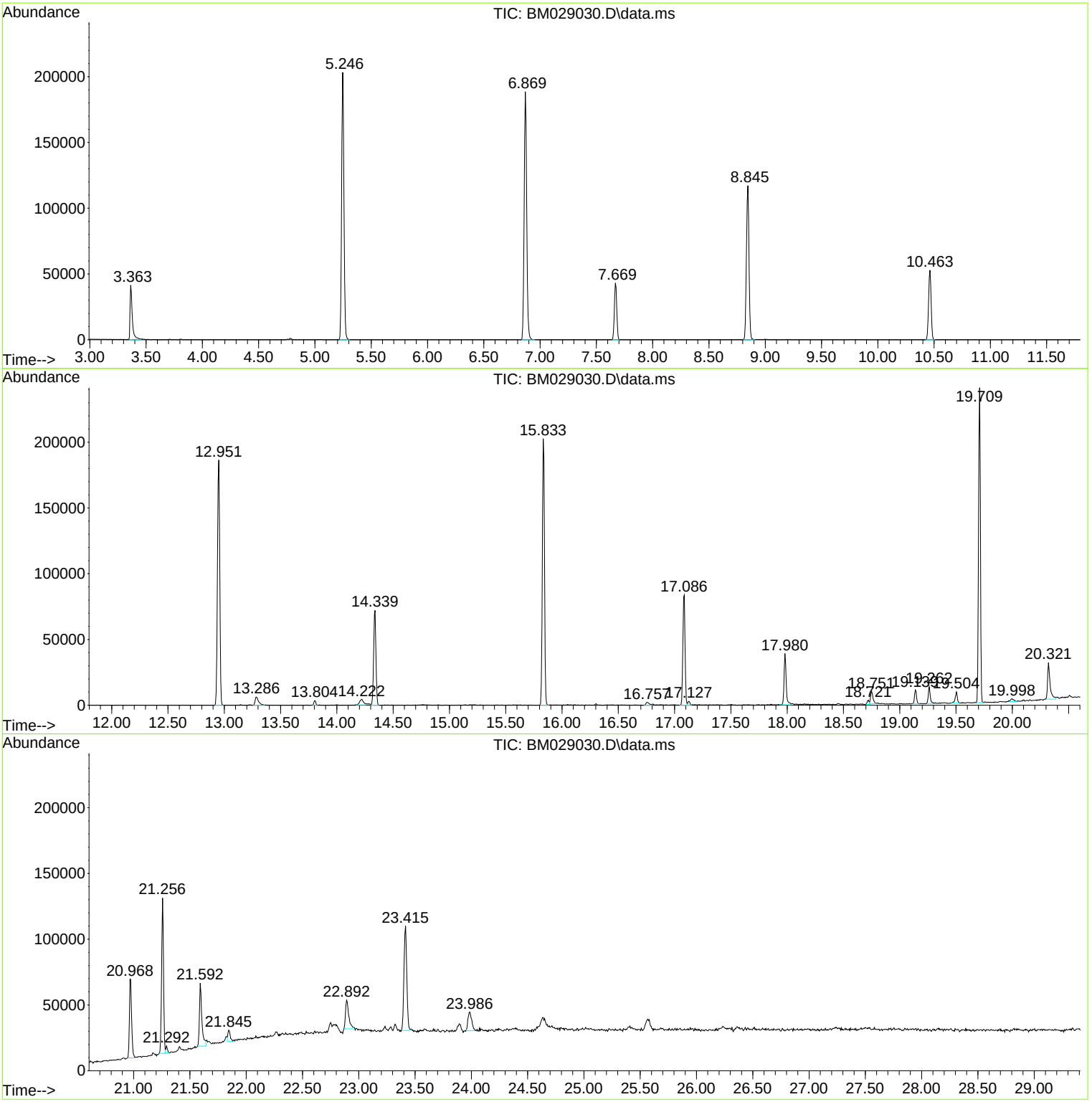
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
RO-363

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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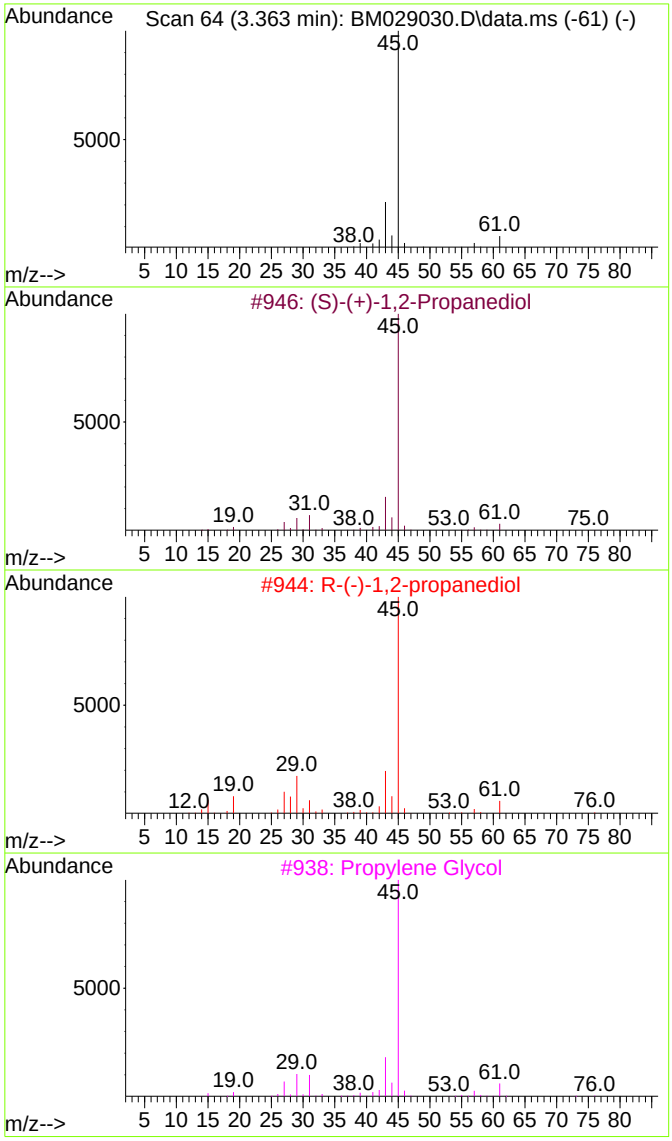
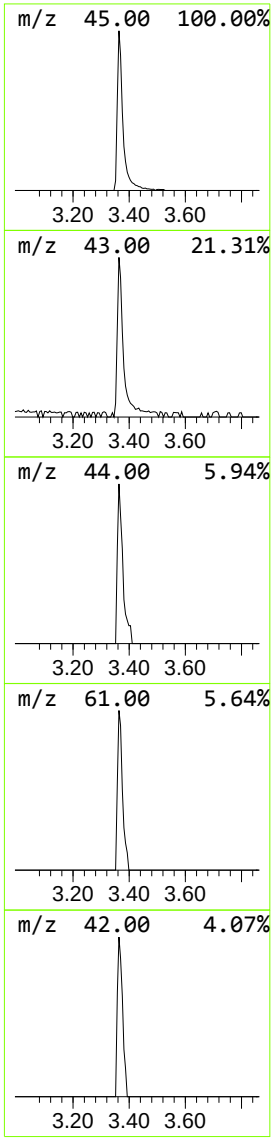
Peak Number 1 (S)-(+)-1,2-Propanediol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.363	18.17 ng	56891	1,4-Dichlorobenzene-d4	7.669

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	64
2	R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	43
3	Propylene Glycol	76	C3H8O2	000057-55-6	9
4	Isopropyl Alcohol	60	C3H8O	000067-63-0	9
5	Formamide	45	CH3NO	000075-12-7	5





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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM022321.M
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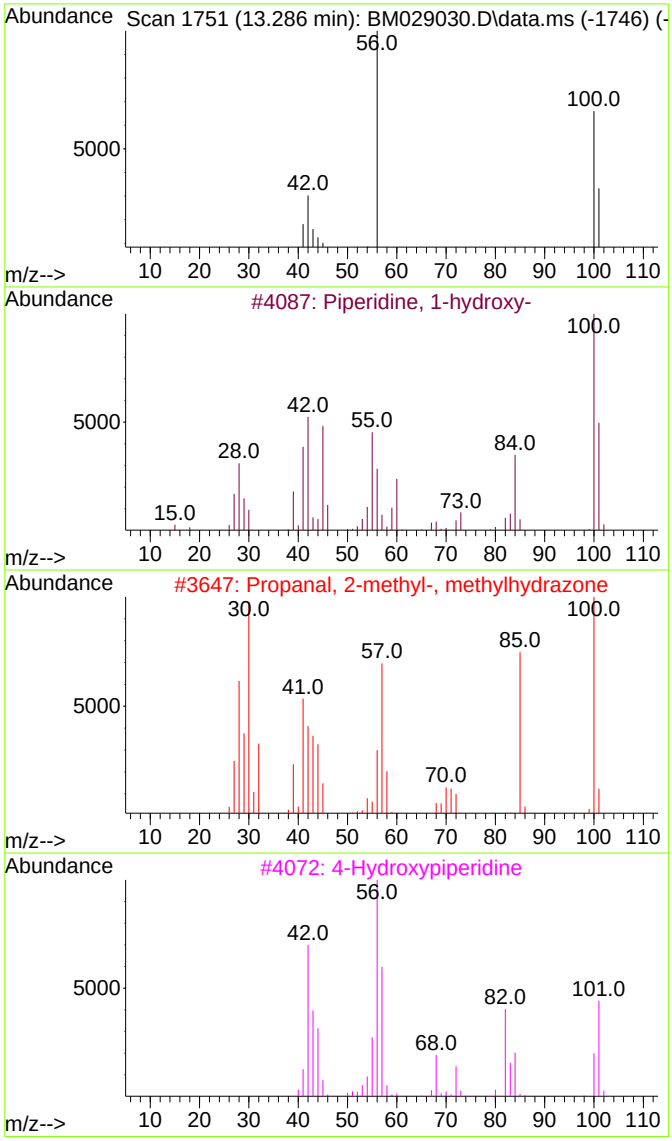
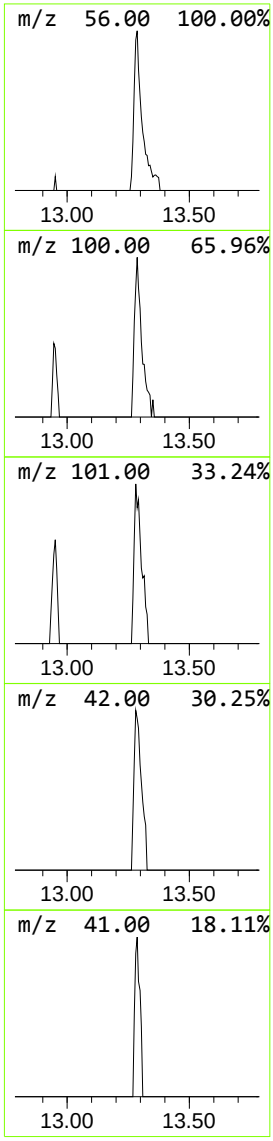
Peak Number 2 unknown13.286 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.286	2.68 ng	13710	Acenaphthene-d10	14.339

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Piperidine, 1-hydroxy-	101	C5H11NO	004801-58-5	38
2	Propanal, 2-methyl-, methylhydra...	100	C5H12N2	016713-37-4	9
3	4-Hydroxypiperidine	101	C5H11NO	005382-16-1	9
4	2-Piperazinone	100	C4H8N2O	005625-67-2	9
5	Propanenitrile, 2-hydroxy-	71	C3H5NO	000078-97-7	9





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ClientSampleId :
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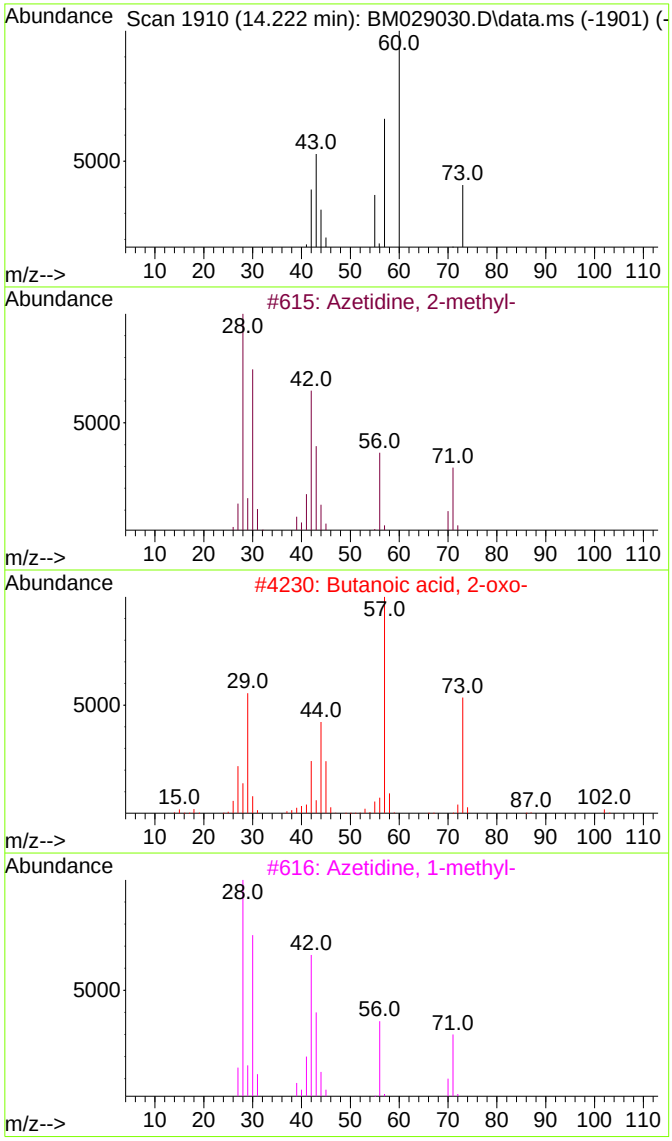
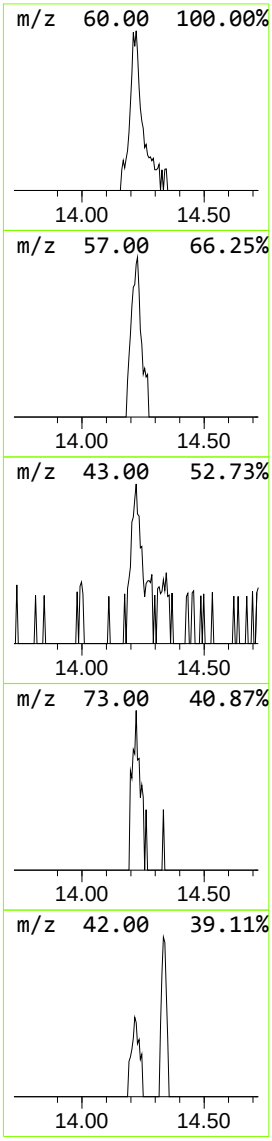
Peak Number 3 unknown14.222 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.222	2.01 ng	10313	Acenaphthene-d10	14.339

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Azetidine, 2-methyl-	71	C4H9N	019812-49-8	9
2	Butanoic acid, 2-oxo-	102	C4H6O3	000600-18-0	9
3	Azetidine, 1-methyl-	71	C4H9N	004923-79-9	7
4	Acetic acid	60	C2H4O2	000064-19-7	7
5	Formic acid hydrazide	60	CH4N2O	000624-84-0	4





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Instrument :
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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
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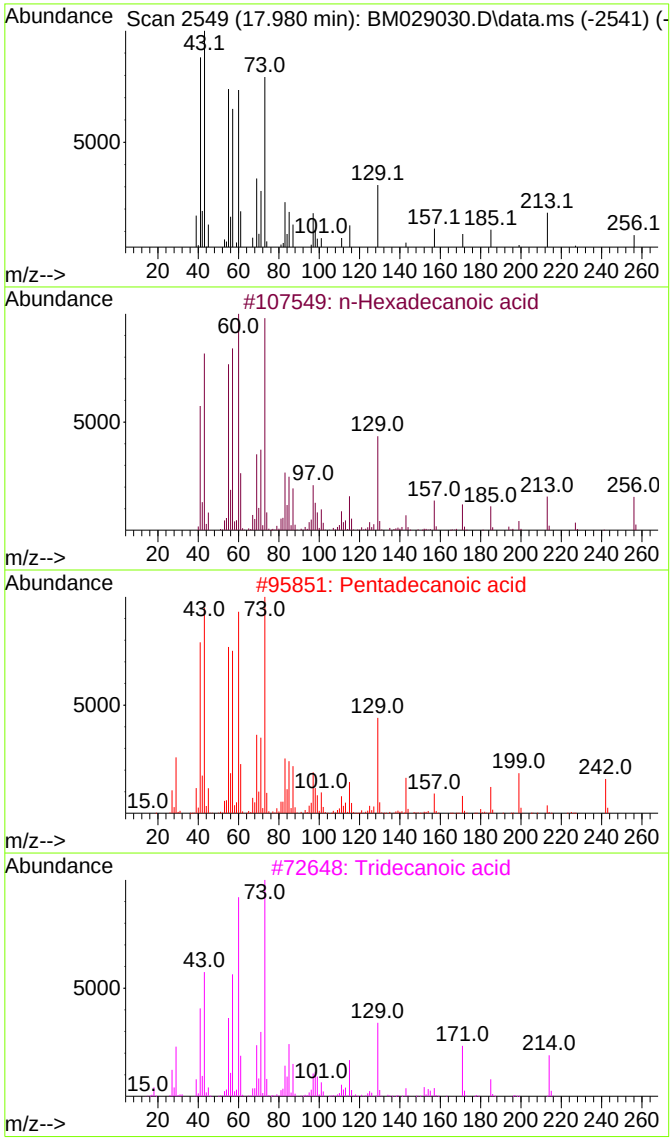
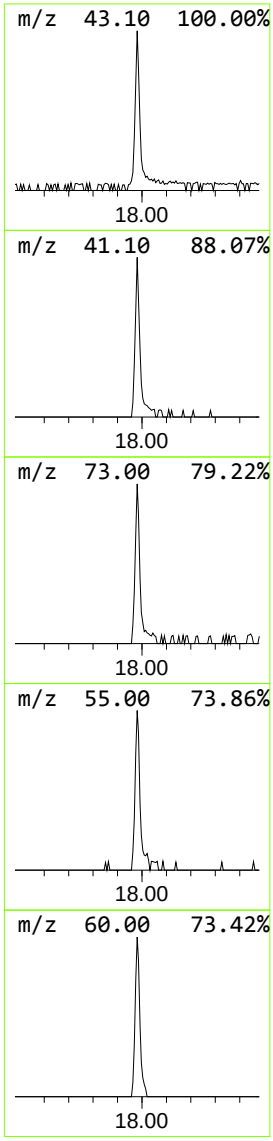
Peak Number 4 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.980	8.81 ng	50109	Phenanthrene-d10	17.086

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	91
3	Tridecanoic acid	214	C13H26O2	000638-53-9	80
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	72
5	n-Decanoic acid	172	C10H20O2	000334-48-5	53





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Instrument : BNA_M
ClientSampleId : RO-363

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM022321.M
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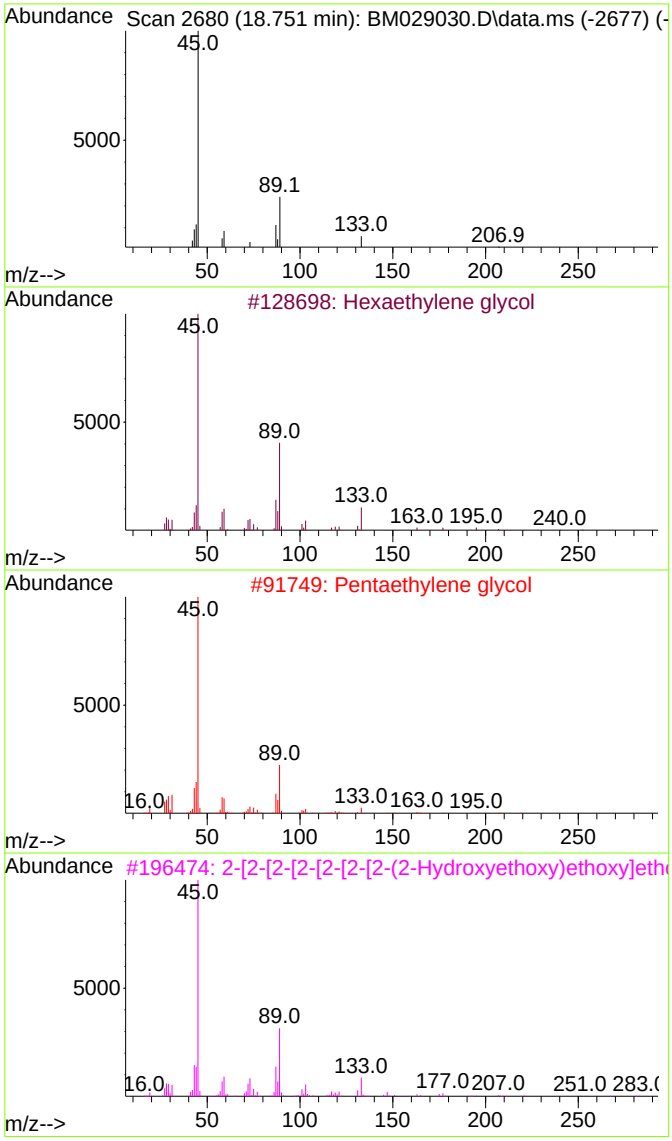
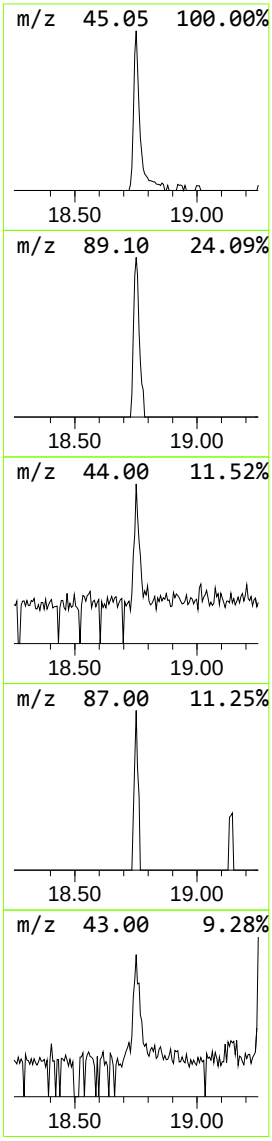
Peak Number 5 Hexaethylene glycol Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.751	2.38 ng	13546	Phenanthrene-d10	17.086

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexaethylene glycol	282	C12H26O7	002615-15-8	83
2	Pentaethylene glycol	238	C10H22O6	004792-15-8	78
3	2-[2-[2-[2-[2-[2-(2-Hydroxyet...	370	C16H34O9	005117-19-1	74
4	2,5,8,11,14-Pentaoxahexadecan-16-ol	252	C11H24O6	023778-52-1	74
5	Tetraethylene glycol	194	C8H18O5	000112-60-7	43





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TIC Library : C:\DATABASE\NIST11.L
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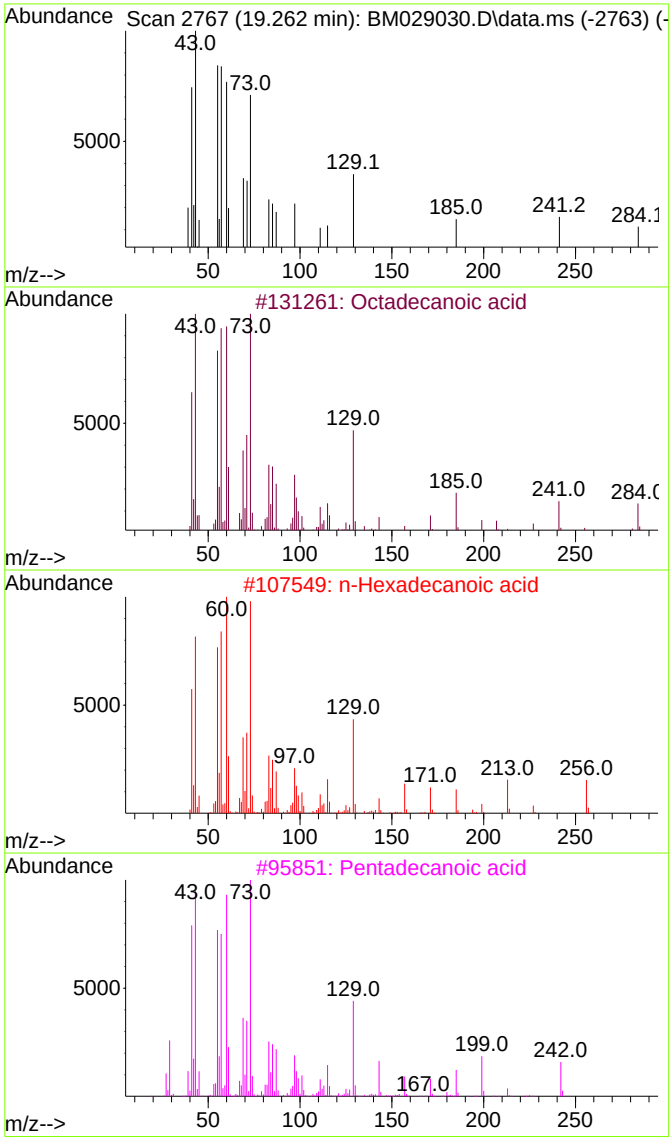
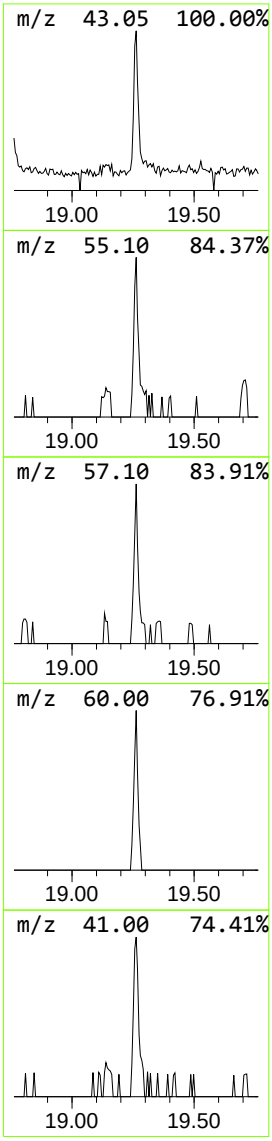
Peak Number 6 Octadecanoic acid Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.262	2.26 ng	15914	Chrysene-d12	21.256

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	98
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	83
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	72
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	64
5	Dodecanoic acid	200	C12H24O2	000143-07-7	59





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
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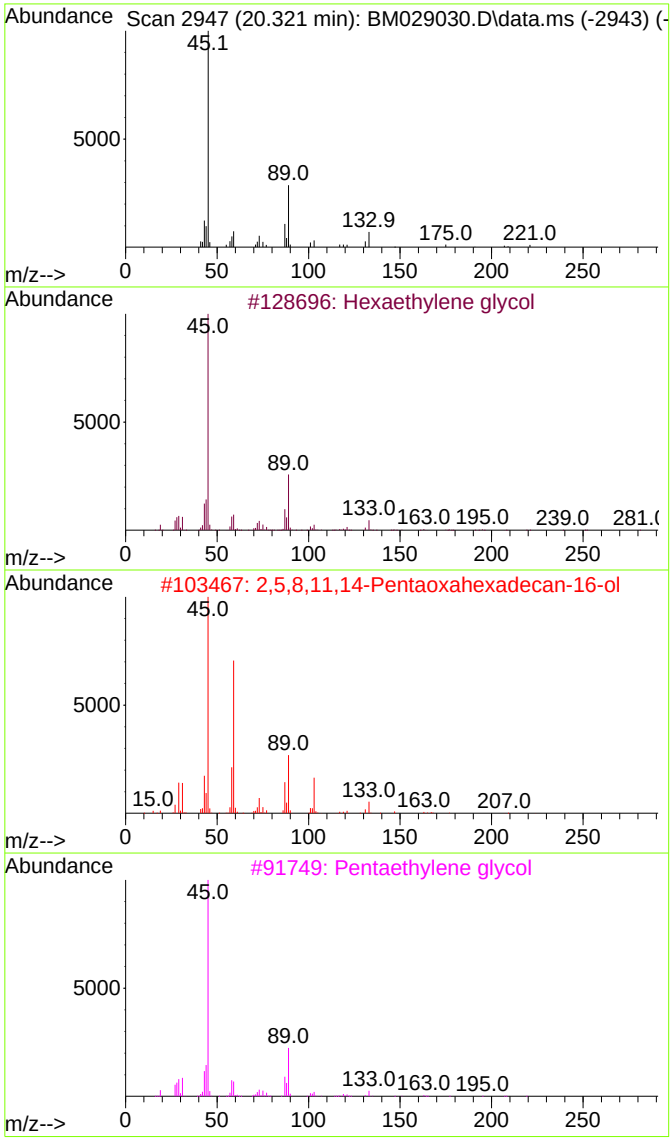
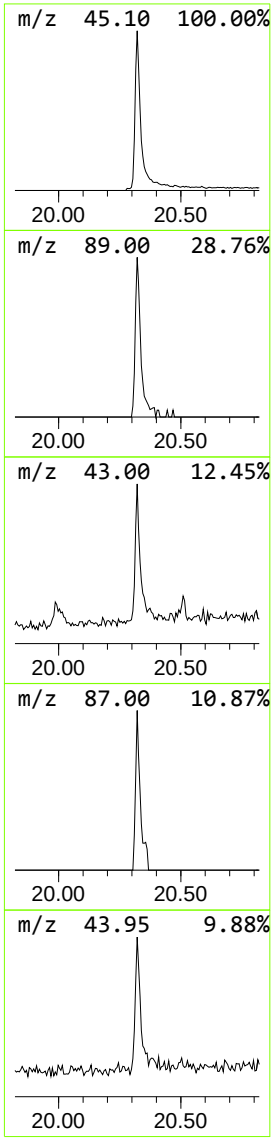
Peak Number 7 2,5,8,11,14-Pentaoxahexadec... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.321	6.01 ng	42371	Chrysene-d12	21.256

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexaethylene glycol	282	C12H26O7	002615-15-8	86
2	2,5,8,11,14-Pentaoxahexadecan-16-ol	252	C11H24O6	023778-52-1	83
3	Pentaethylene glycol	238	C10H22O6	004792-15-8	72
4	Triethylene glycol	150	C6H14O4	000112-27-6	72
5	Tetraethylene glycol	194	C8H18O5	000112-60-7	64





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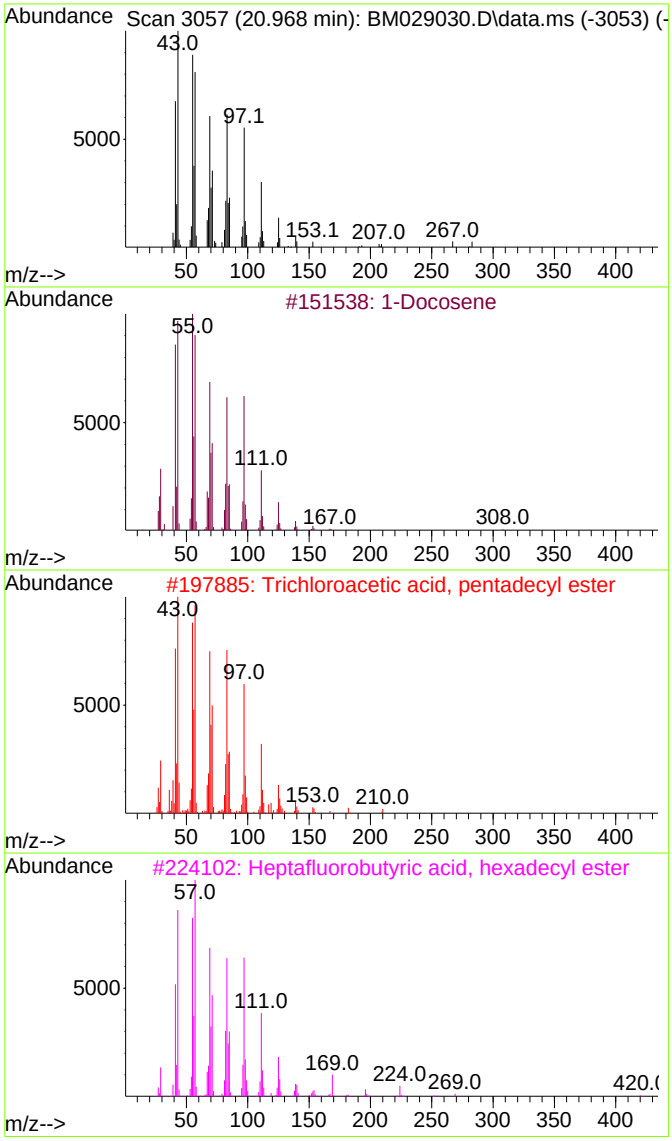
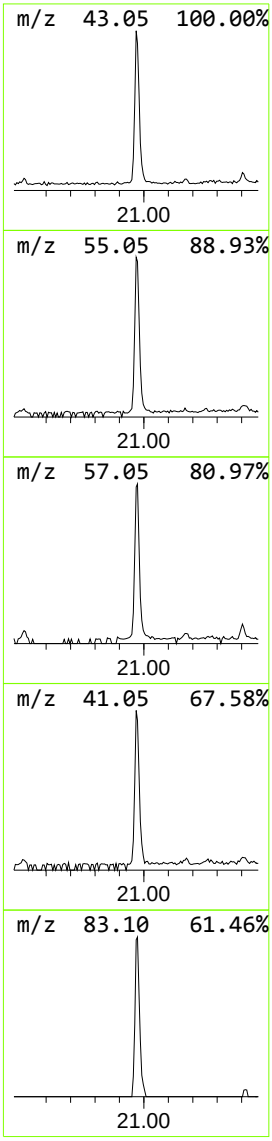
Peak Number 8 1-Docosene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.968	11.49 ng	80979	Chrysene-d12	21.256

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Docosene	308	C22H44	001599-67-3	95
2	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	94
3	Heptafluorobutyric acid, hexadec...	438	C20H33F7O2	006385-15-5	94
4	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	94
5	Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	94





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

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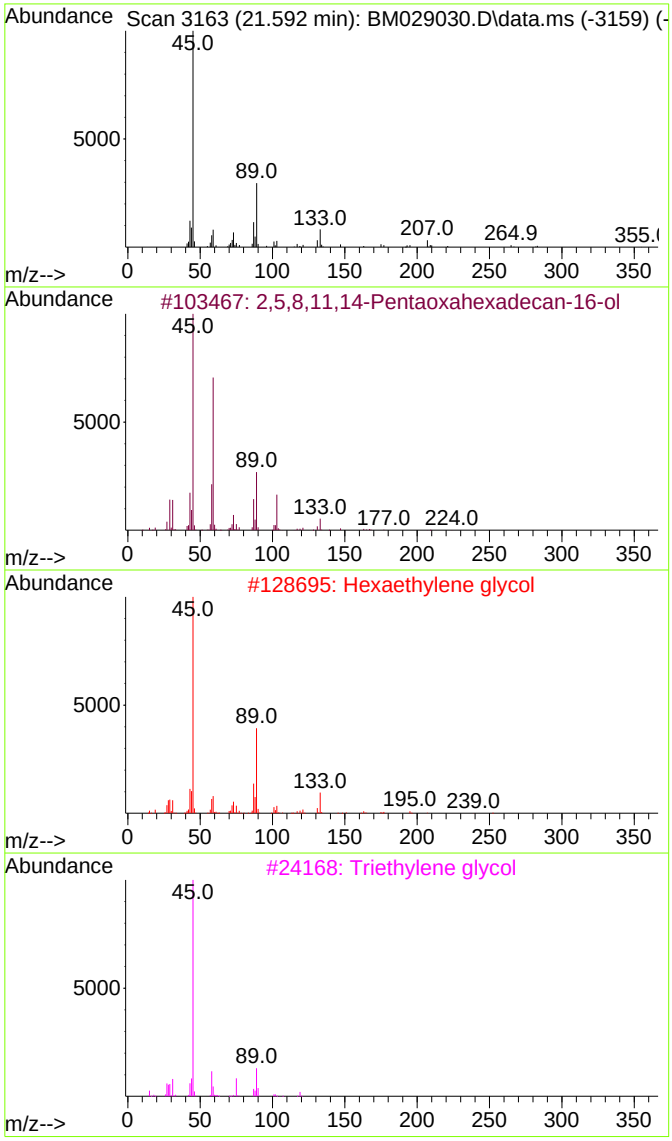
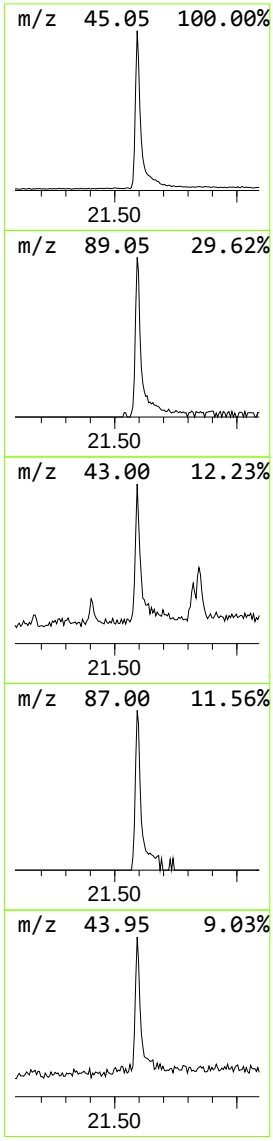
Peak Number 9 Triethylene glycol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.592	10.37 ng	73043	Chrysene-d12	21.256

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,5,8,11,14-Pentaoxahexadecan-16-ol	252	C11H24O6	023778-52-1	90
2	Hexaethylene glycol	282	C12H26O7	002615-15-8	83
3	Triethylene glycol	150	C6H14O4	000112-27-6	78
4	Tetraethylene glycol	194	C8H18O5	000112-60-7	78
5	Pentaethylene glycol	238	C10H22O6	004792-15-8	74





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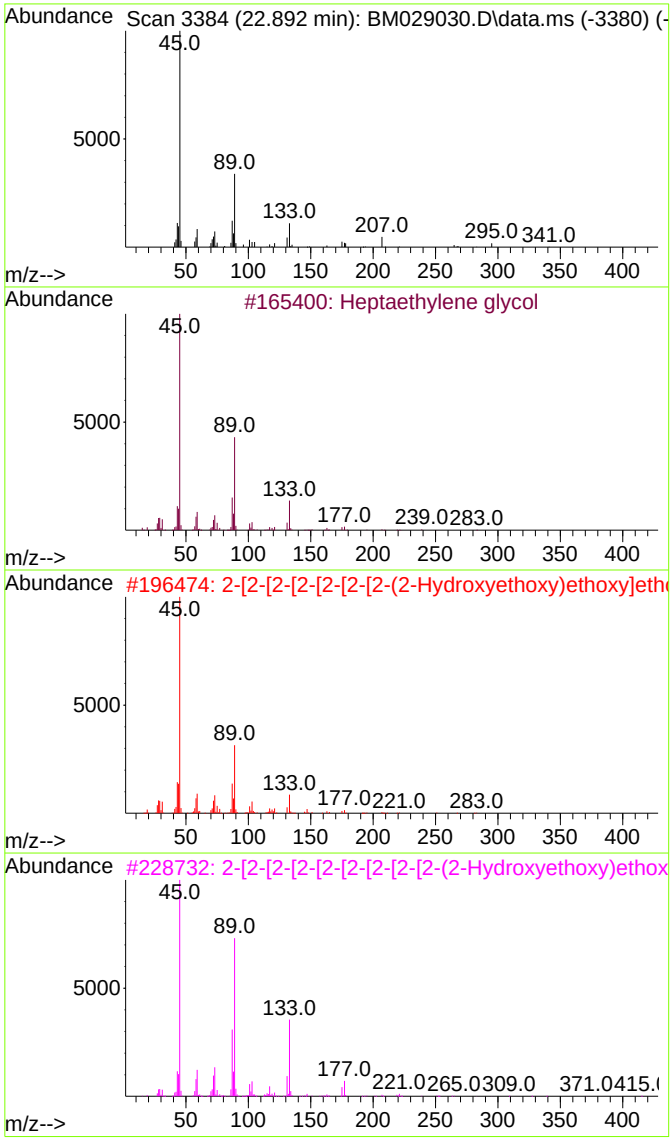
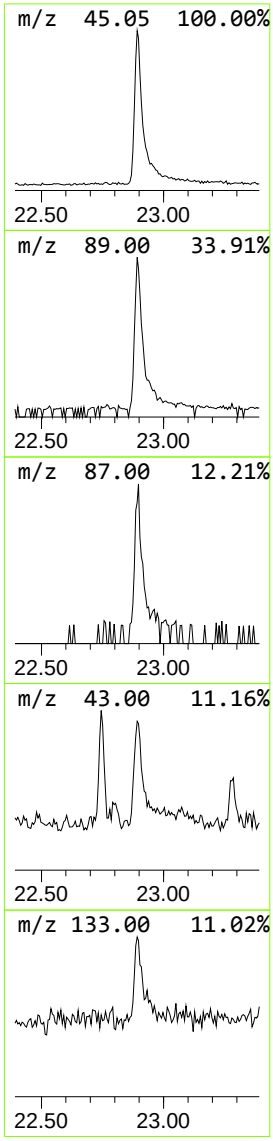
Peak Number 10 Heptaethylene glycol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.892	6.33 ng	43778	Perylene-d12	23.415

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptaethylene glycol	326	C14H30O8	005617-32-3	90
2	2-[2-[2-[2-[2-[2-(2-Hydroxyet...	370	C16H34O9	005117-19-1	86
3	2-[2-[2-[2-[2-[2-[2-[2-(2-Hyd...	458	C20H42O11	1000352-12-6	78
4	Hexaethylene glycol	282	C12H26O7	002615-15-8	72
5	2,5,8,11,14-Pentaoxahexadecan-16-ol	252	C11H24O6	023778-52-1	72





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM030821\
Data File : BM029030.D
Acq On : 08 Mar 2021 21:57
Operator : CG/JU
Sample : M1582-03
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
RO-363

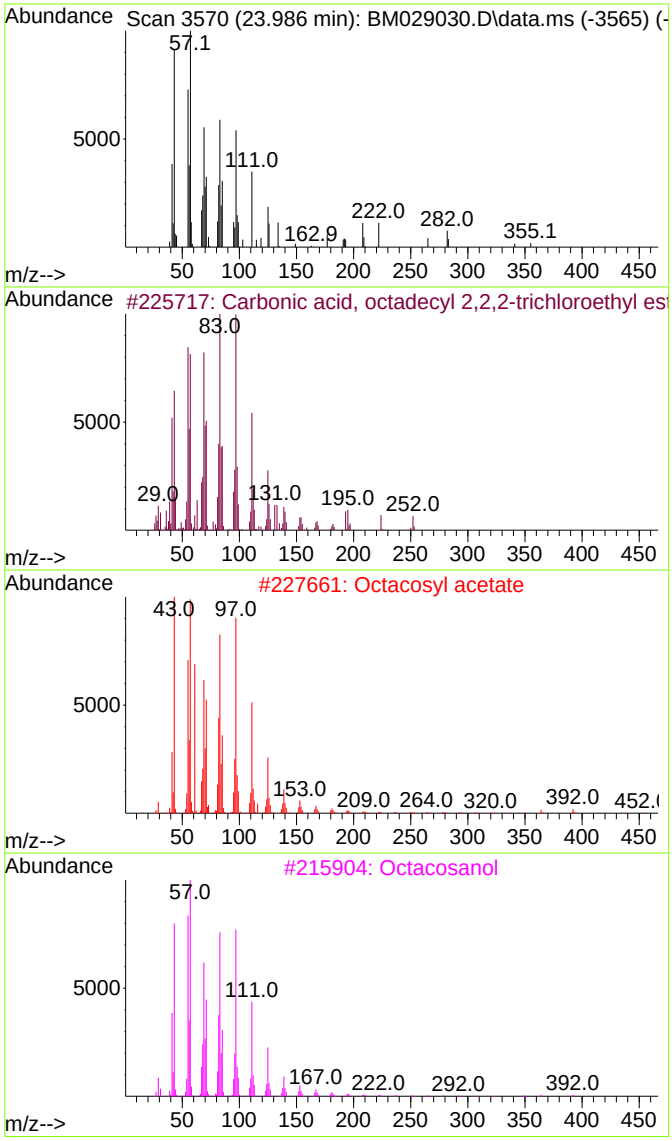
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM022321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

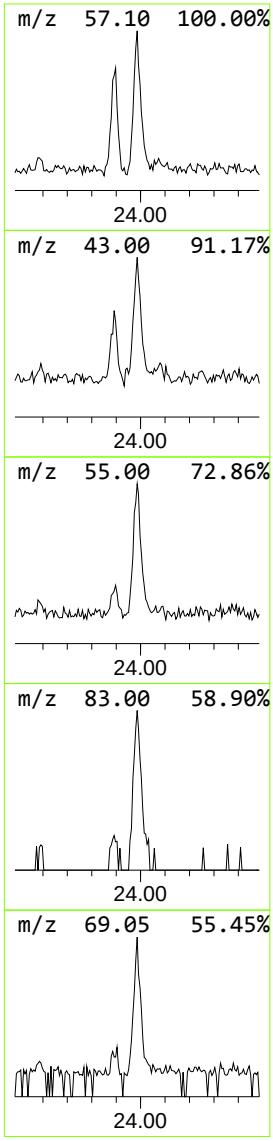
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 11 Carbonic acid, octadecyl 2,... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.986	4.69 ng	32472	Perylene-d12	23.415

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Carbonic acid, octadecyl 2,2,2-t...	444	C21H39Cl3O3	1000314-56-3	81
2	Octacosyl acetate	452	C30H60O2	018206-97-8	74
3	Octacosanol	410	C28H58O	000557-61-9	74
4	1-Tricosene	322	C23H46	018835-32-0	74
5	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	74





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM030821\
Data File : BM029030.D
Acq On : 08 Mar 2021 21:57
Operator : CG/JU
Sample : M1582-03
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : RO-363

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
(S)-(+)-1,2-Pro...	3.363	18.2	ng	56891	1	7.669	62611	20.0
unknown13.286	13.286	2.7	ng	13710	3	14.339	102400	20.0
unknown14.222	14.222	2.0	ng	10313	3	14.339	102400	20.0
n-Hexadecanoic ...	17.980	8.8	ng	50109	4	17.086	113766	20.0
Hexaethylene gl...	18.751	2.4	ng	13546	4	17.086	113766	20.0
Octadecanoic acid	19.262	2.3	ng	15914	5	21.256	140906	20.0
2,5,8,11,14-Pen...	20.321	6.0	ng	42371	5	21.256	140906	20.0
1-Docosene	20.968	11.5	ng	80979	5	21.256	140906	20.0
Triethylene glycol	21.592	10.4	ng	73043	5	21.256	140906	20.0
Heptaethylene g...	22.892	6.3	ng	43778	6	23.415	138358	20.0
Carbonic acid, ...	23.986	4.7	ng	32472	6	23.415	138358	20.0