LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF032921\
Data File : BF123502.D
Acq On : 29 Mar 2021 18:43
Operator : JU/CG
Sample : M1813-03
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : VNJ-236

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-BF032321.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF123502.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.240	17	26	32	rVB	1239536	1562716	17.04%	2.531%
2	2.346	38	44	51	rVB	192368	244787	2.67%	0.396%
3	3.628	228	262	265	rBV	1311158	9169924	100.00%	14.852%
4	5.122	512	516	522	rVB	281484	302280	3.30%	0.490%
5	5.522	579	584	588	rBV	4378579	4489192	48.96%	7.271%
6	6.528	749	755	758	rBV	4091166	4560545	49.73%	7.387%
7	6.898	814	818	821	rBV	2073425	1636877	17.85%	2.651%
8	7.457	908	913	916	rBV	3092002	2931430	31.97%	4.748%
9	8.181	1032	1036	1040	rBV	2359769	2132620	23.26%	3.454%
10	9.263	1214	1220	1223	rBV	4733515	4540788	49.52%	7.355%
11	9.416	1237	1246	1265	rBV	809939	1549643	16.90%	2.510%
12	9.898	1325	1328	1329	rBV	97710	109306	1.19%	0.177%
13	9.939	1329	1335	1339	rVB	2628026	2538582	27.68%	4.112%
14	10.727	1464	1469	1473	rBV	3353105	3087931	33.67%	5.001%
15	11.245	1553	1557	1563	rBV	162814	346578	3.78%	0.561%
16	11.433	1584	1589	1592	rBV	2564844	2326920	25.38%	3.769%
17	11.957	1672	1678	1690	rBV	659413	717675	7.83%	1.162%
18	12.421	1753	1757	1788	rBV2	517049	1874761	20.44%	3.036%
19	12.745	1808	1812	1822	rVB	103121	141128	1.54%	0.229%
20	13.021	1855	1859	1862	rBV	4919983	4304453	46.94%	6.972%
21	13.451	1929	1932	1955	rBV	1118361	2843406	31.01%	4.605%
22	13.780	1985	1988	1994	rVB	131406	126115	1.38%	0.204%
23	13.939	2011	2015	2030	rVB2	440502	909492	9.92%	1.473%
24	14.080	2033	2039	2042	rBV	1511439	1527381	16.66%	2.474%
25	14.368	2084	2088	2100	rBV	1717647	3048442	33.24%	4.937%
26	14.580	2122	2124	2134	rVB3	69929	155986	1.70%	0.253%
27	15.315	2244	2249	2276	rBV	455345	2674872	29.17%	4.332%
28	15.574	2288	2293	2298	rBV	1075072	1352664	14.75%	2.191%
29	16.192	2391	2398	2411	rVB6	59845	214120	2.34%	0.347%
30	16.609	2462	2469	2472	rBV5	140362	320877	3.50%	0.520%

Sum of corrected areas: 61741491

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Misc :
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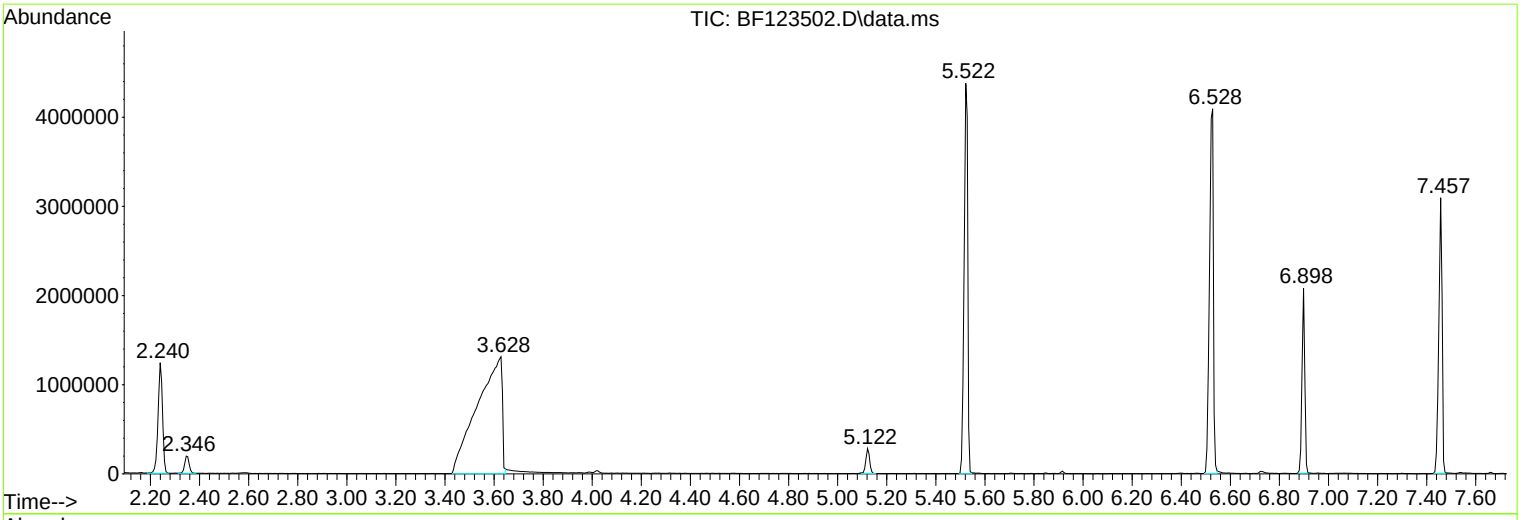
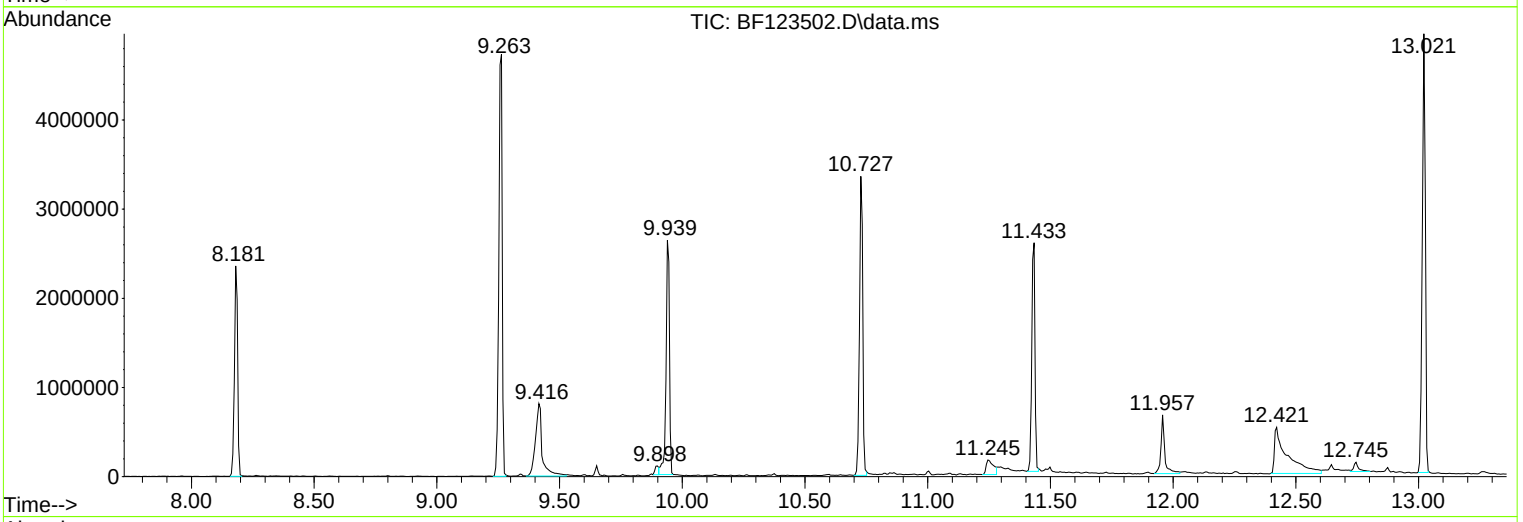
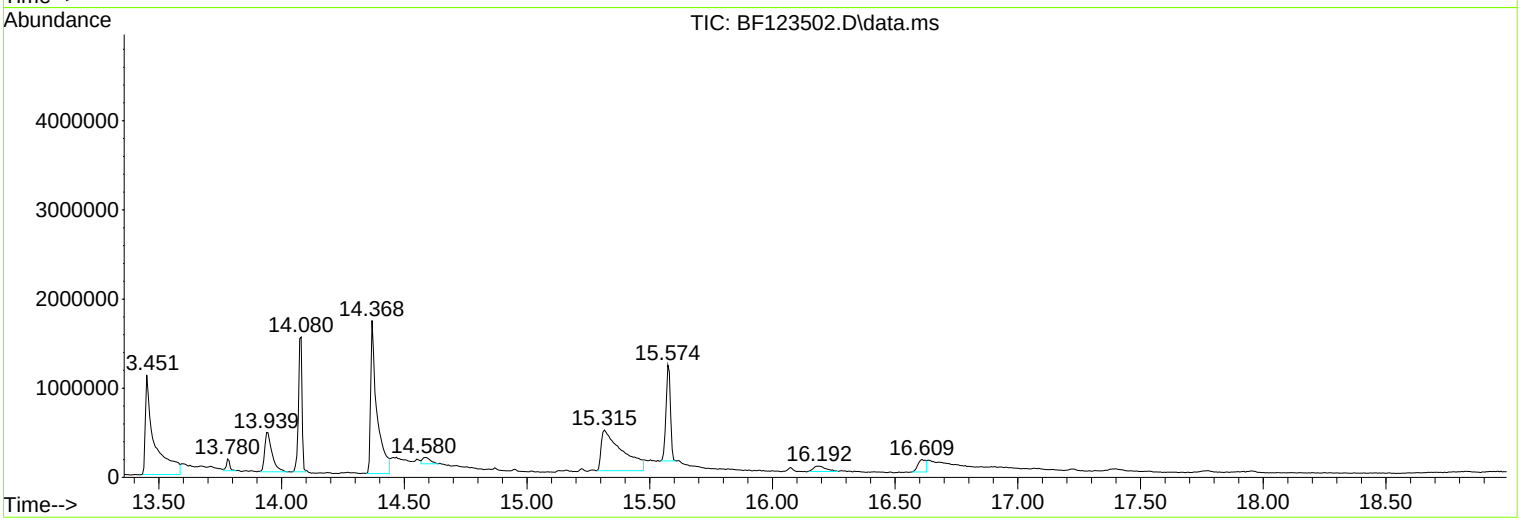
Instrument :
BNA_F
ClientSampleId :
VNJ-236

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF032321.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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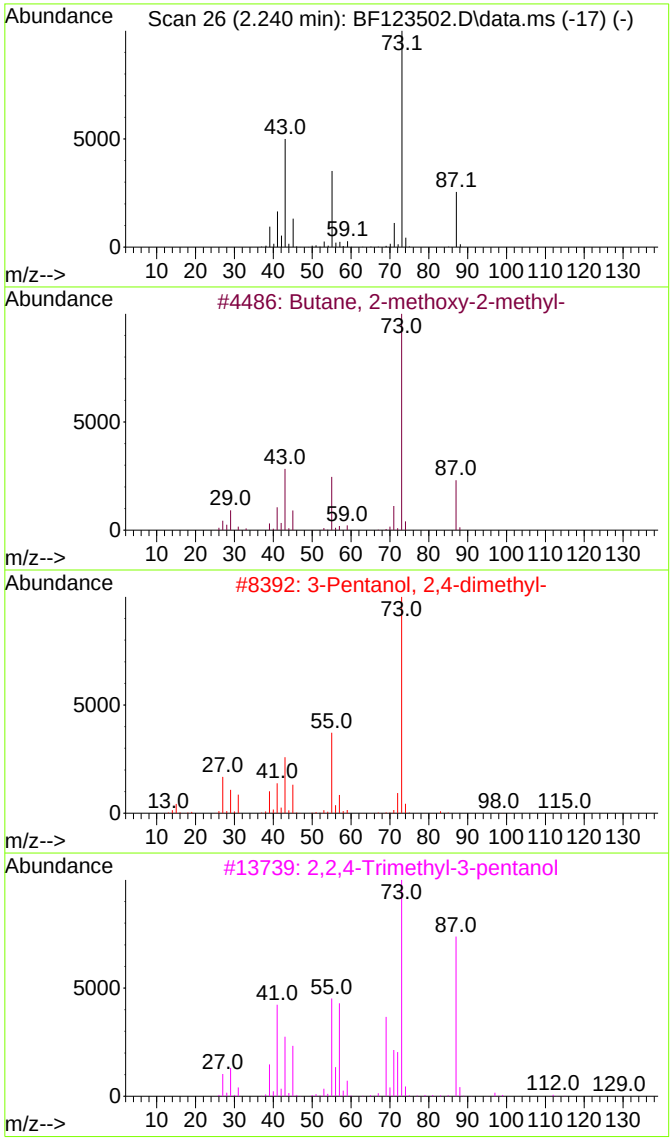
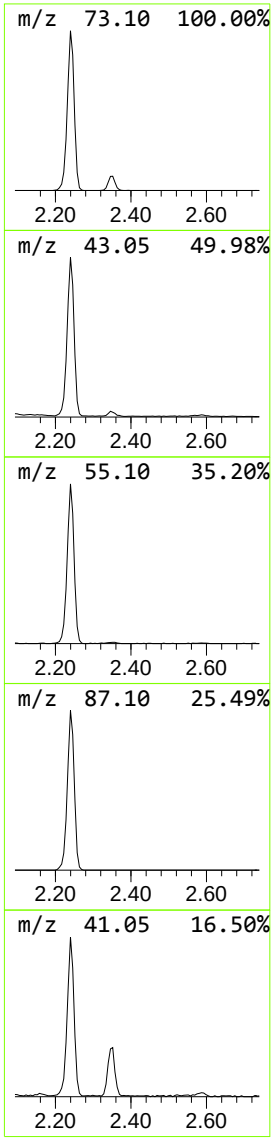
****
Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.240	19.09 ng	1562720	1,4-Dichlorobenzene-d4	6.898

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2	3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	43
3	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
4	Silane, tetramethyl-	88	C4H12Si	000075-76-3	38
5	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	23





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Operator : JU/CG
Sample : M1813-03
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Instrument : BNA_F
ClientSampleId : VNJ-236

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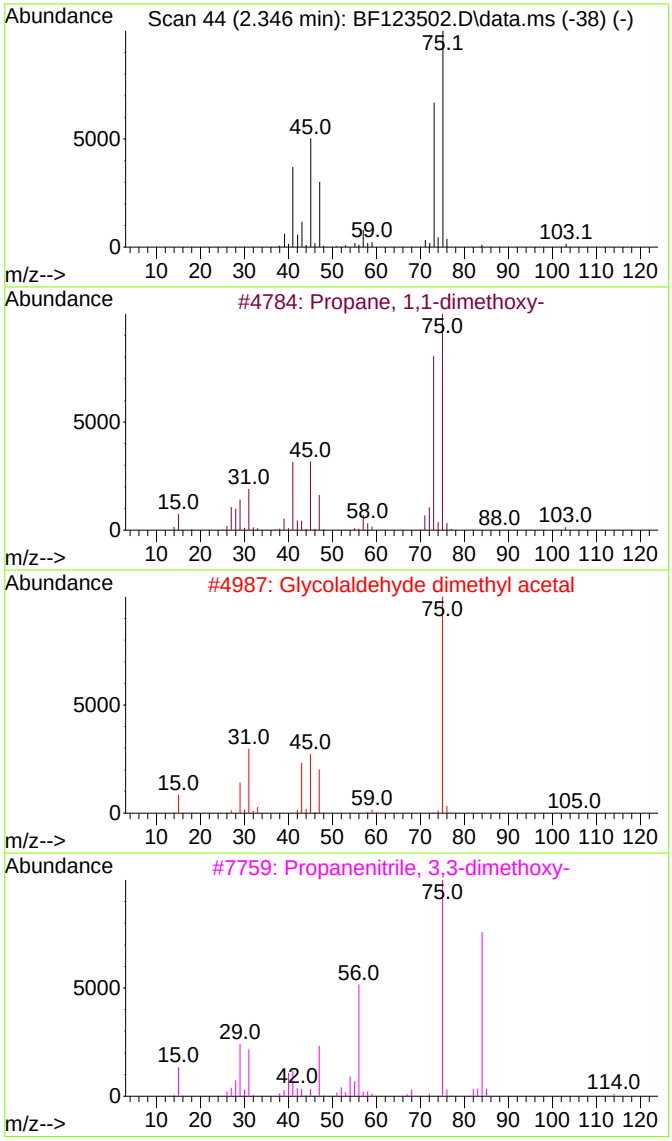
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

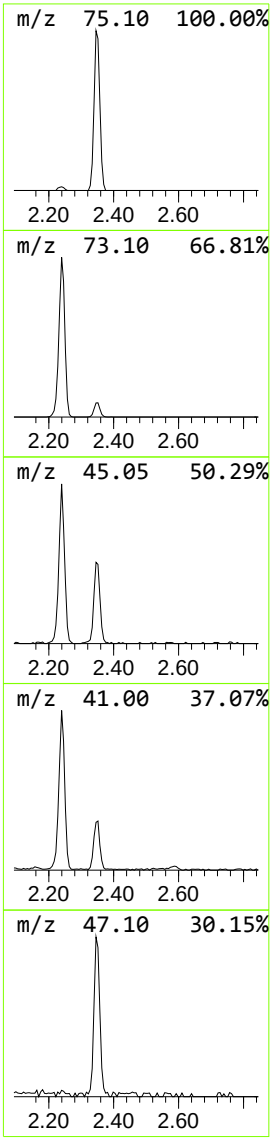
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Propane, 1,1-dimethoxy- Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.346	2.99 ng	244787	1,4-Dichlorobenzene-d4	6.898

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 1,1-dimethoxy-	104	C5H12O2	004744-10-9	64
2	Glycolaldehyde dimethyl acetal	106	C4H10O3	030934-97-5	38
3	Propanenitrile, 3,3-dimethoxy-	115	C5H9NO2	057597-62-3	38
4	Aminoacetaldehyde dimethyl acetal	105	C4H11NO2	022483-09-6	33
5	Methane, trimethoxy-	106	C4H10O3	000149-73-5	33





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Operator : JU/CG
Sample : M1813-03
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : VNJ-236

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF032321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

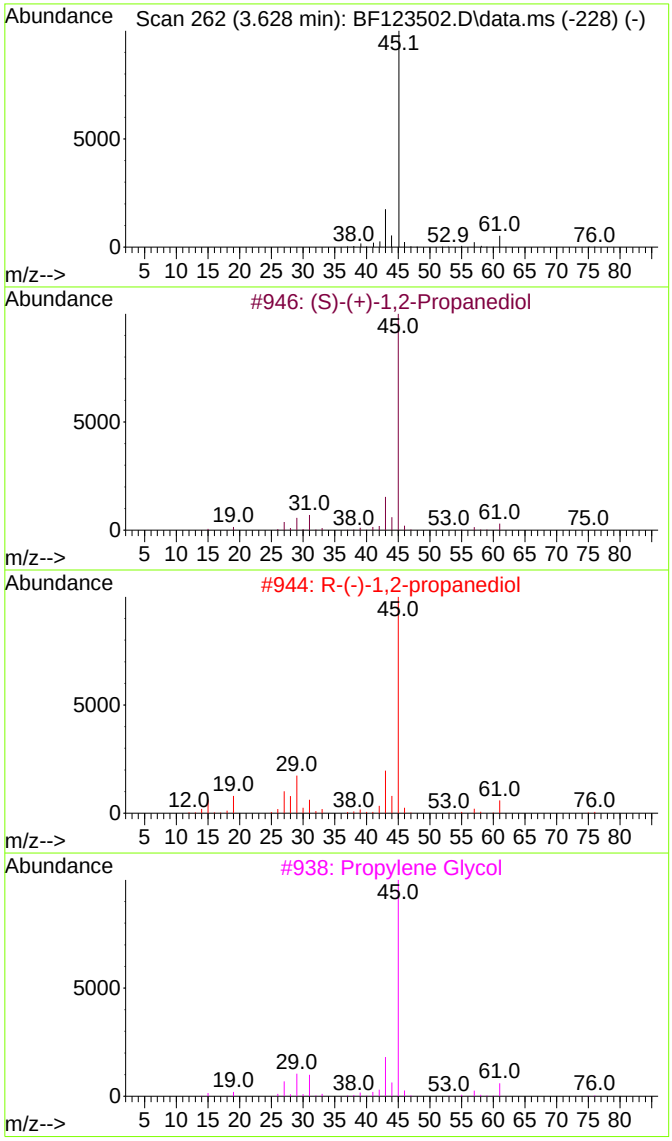
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

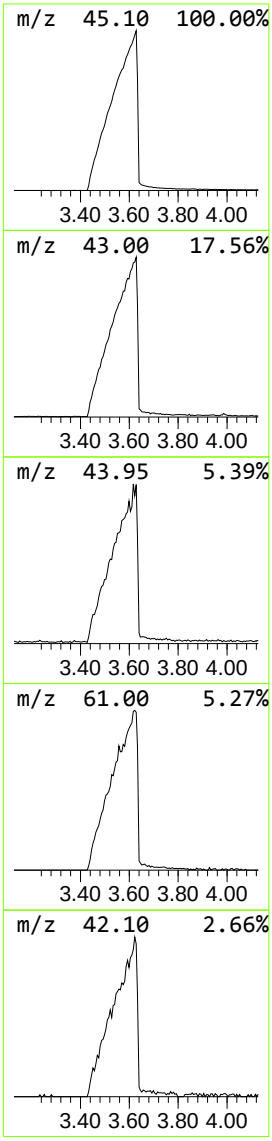
****

Peak Number 3 (S)-(+)-1,2-Propanediol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.628	112.04 ng	9169920	1,4-Dichlorobenzene-d4	6.898

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	43
4	Propanoic acid, 2-hydroxy-, meth...	104	C4H8O3	002155-30-8	9
5	Formamide	45	CH3NO	000075-12-7	7





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Instrument : BNA_F
ClientSampleId : VNJ-236

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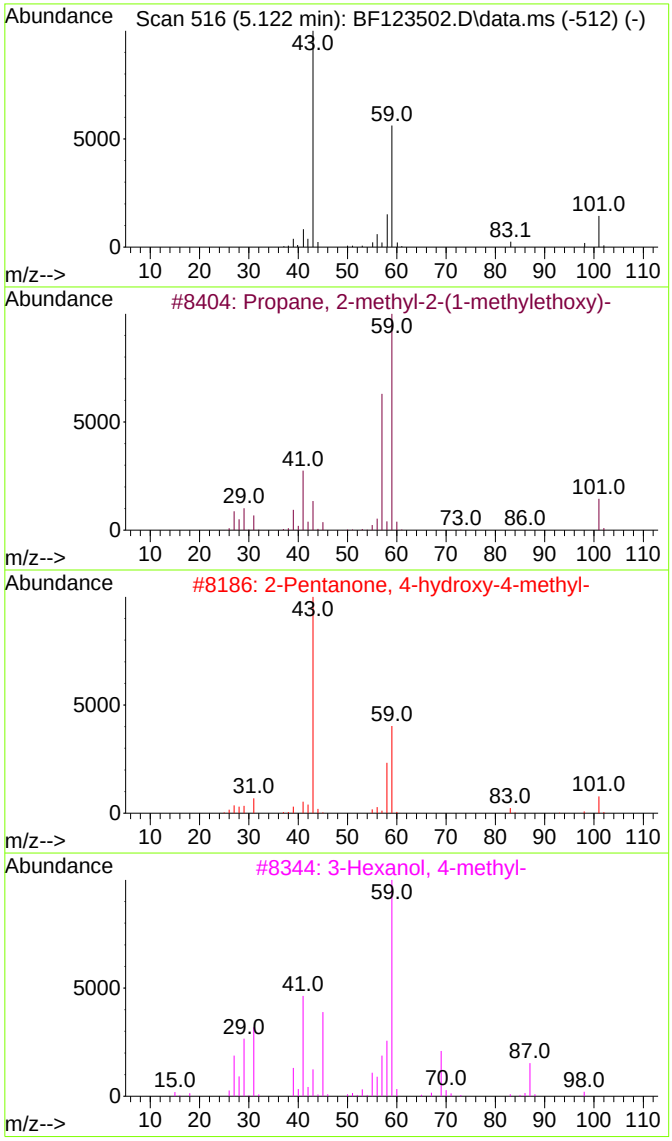
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

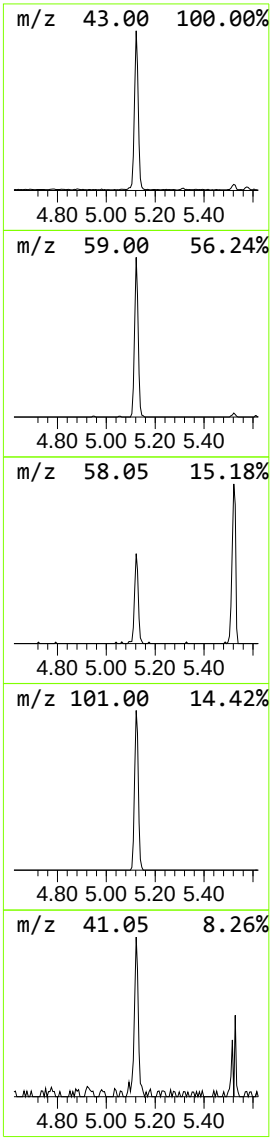
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Propane, 2-methyl-2-(1-meth... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.122	3.69 ng	302280	1,4-Dichlorobenzene-d4	6.898

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	53
2	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
3	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
5	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23





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Sample : M1813-03
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ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : VNJ-236

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF032321.M
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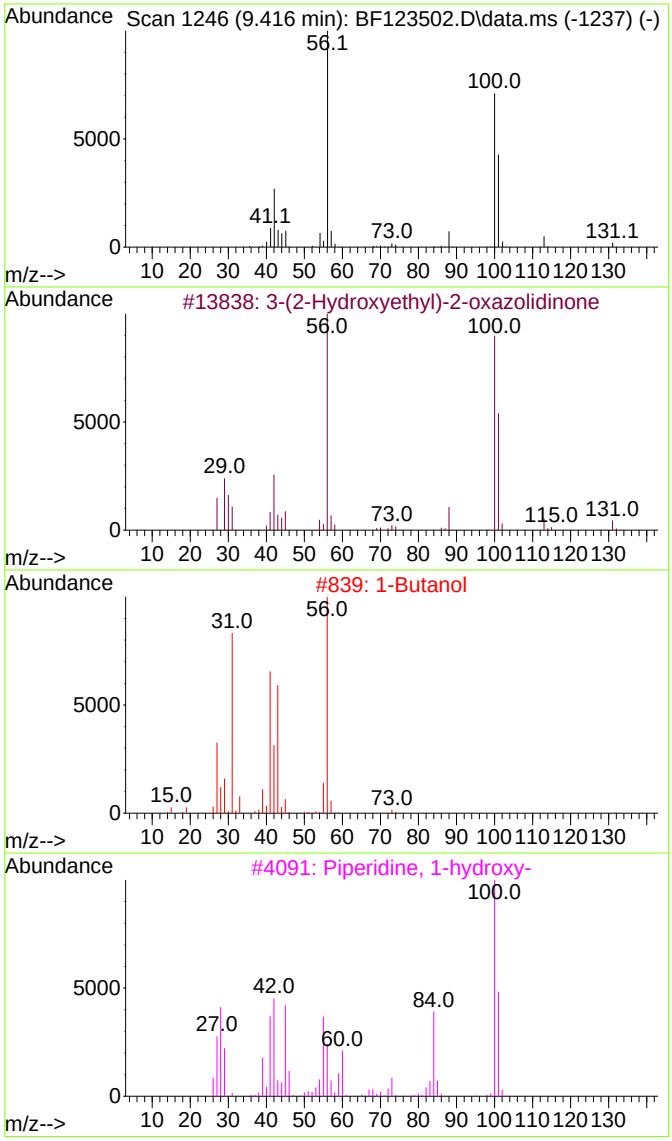
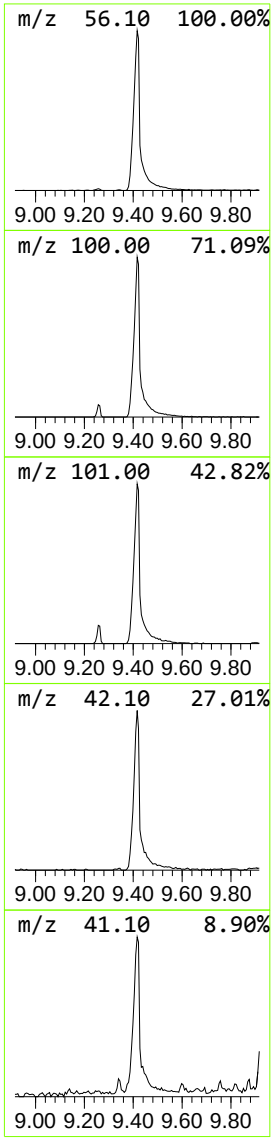
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 3-(2-Hydroxyethyl)-2-oxazol... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.416	12.21 ng	1549640	Acenaphthene-d10	9.939

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-(2-Hydroxyethyl)-2-oxazolidinone	131	C5H9NO3	003356-88-5	56
2	1-Butanol	74	C4H10O	000071-36-3	38
3	Piperidine, 1-hydroxy-	101	C5H11NO	004801-58-5	25
4	Hexyl chloroformate	164	C7H13ClO2	006092-54-2	23
5	4-Morpholineethanol	131	C6H13NO2	000622-40-2	22





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TIC Library : C:\DATABASE\NIST11.L
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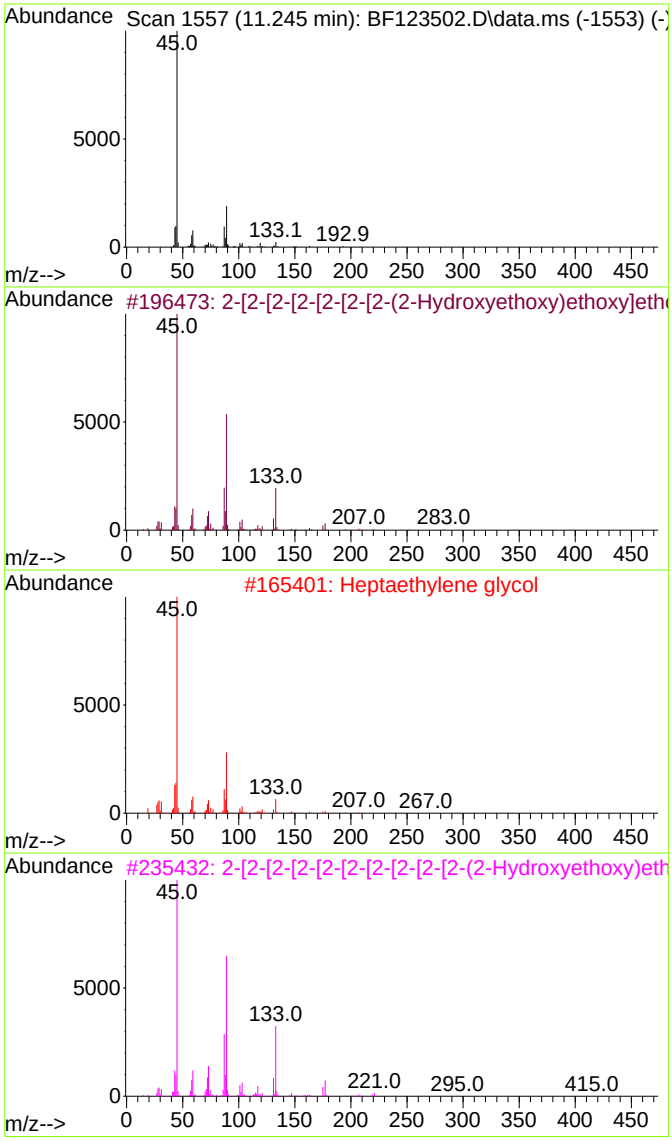
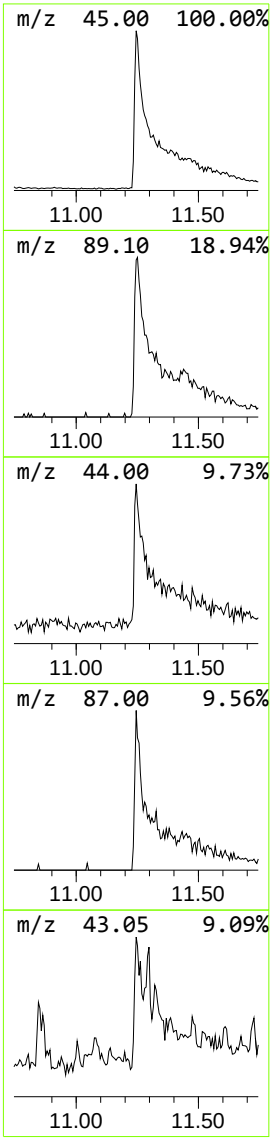
****
Peak Number 6 2-[2-[2-[2-[2-[2-[2-(2-Hydr... Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.245	2.98 ng	346578	Phenanthrene-d10	11.433

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-[2-[2-[2-[2-[2-[2-(2-Hydroxyet...	370	C16H34O9	005117-19-1	83
2	Heptaethylene glycol	326	C14H30O8	005617-32-3	83
3	2-[2-[2-[2-[2-[2-[2-[2-[2-[2-(2-...	502	C22H46O12	1000352-13-2	83
4	2-[2-[2-[2-[2-[2-[2-[2-(2-Hydrox...	414	C18H38O10	1000352-12-5	83
5	Hexaethylene glycol	282	C12H26O7	002615-15-8	83





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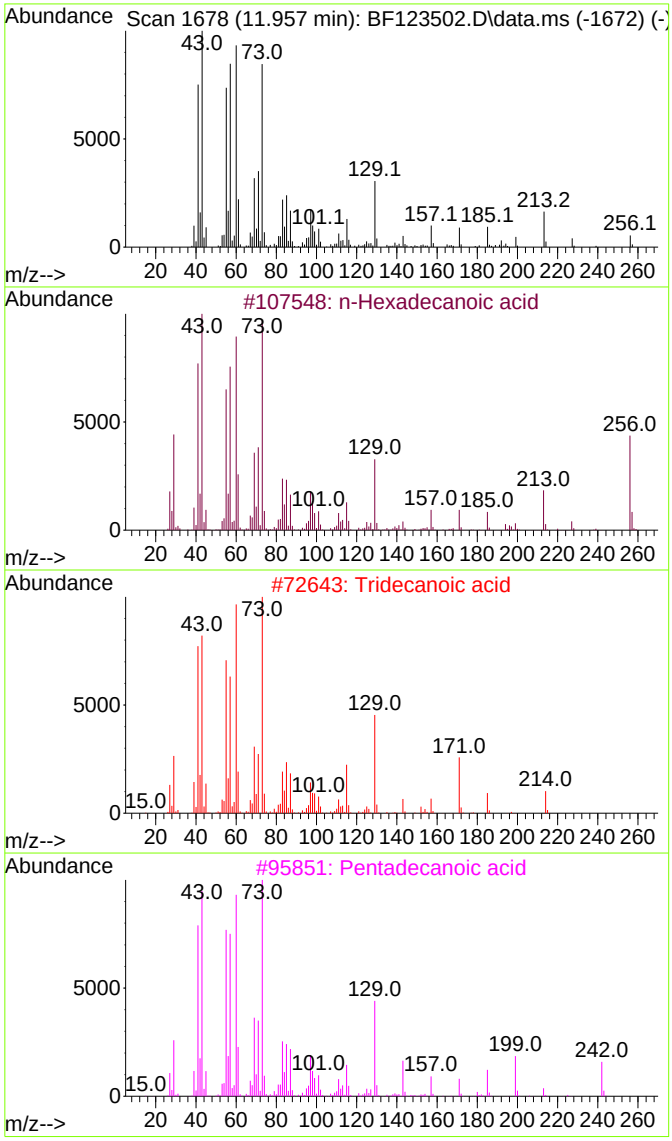
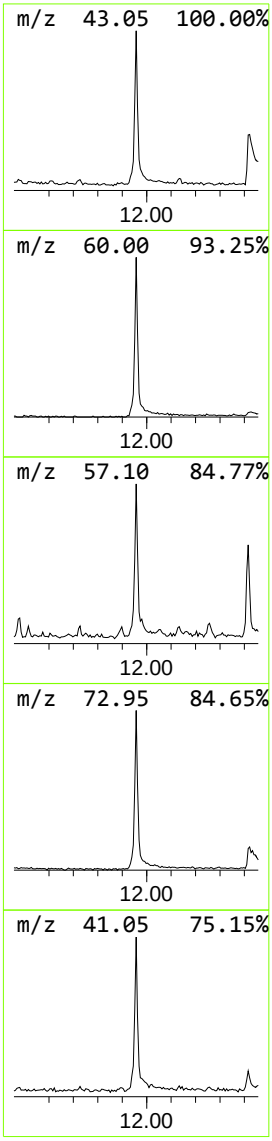
Peak Number 7 n-Hexadecanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.957	6.17 ng	717675	Phenanthrene-d10	11.433

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	94
2	Tridecanoic acid	214	C13H26O2	000638-53-9	93
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	90
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	72
5	Dodecanoic acid	200	C12H24O2	000143-07-7	58





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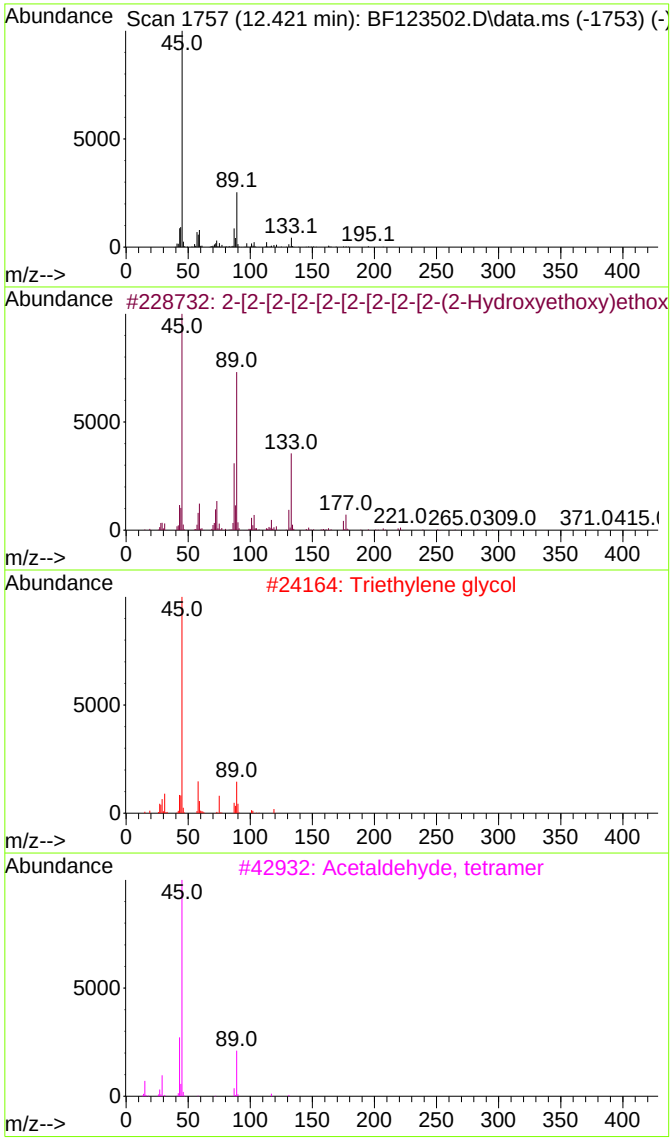
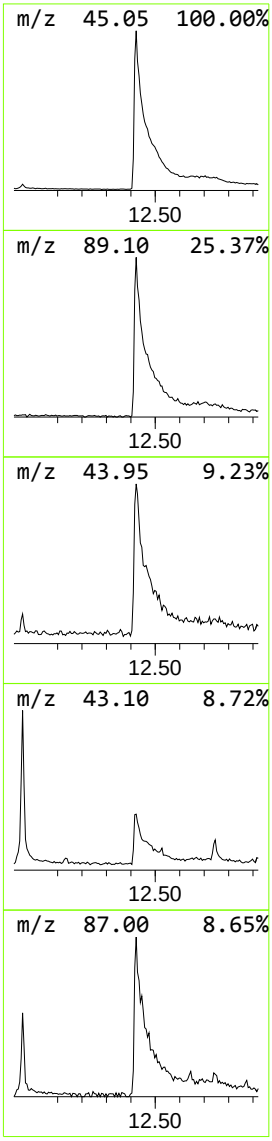
Peak Number 8 Triethylene glycol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.422	16.11 ng	1874760	Phenanthrene-d10	11.433

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-[2-[2-[2-[2-[2-[2-[2-[2-(2-Hyd...	458	C20H42O11	1000352-12-6	83
2	Triethylene glycol	150	C6H14O4	000112-27-6	78
3	Acetaldehyde, tetramer	176	C8H16O4	000108-62-3	72
4	Ethanol, 2-[2-(ethenyloxy)ethoxy]-	132	C6H12O3	000929-37-3	64
5	Hexaethylene glycol	282	C12H26O7	002615-15-8	58





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Operator : JU/CG
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Instrument :
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ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF032321.M
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TIC Library : C:\DATABASE\NIST11.L
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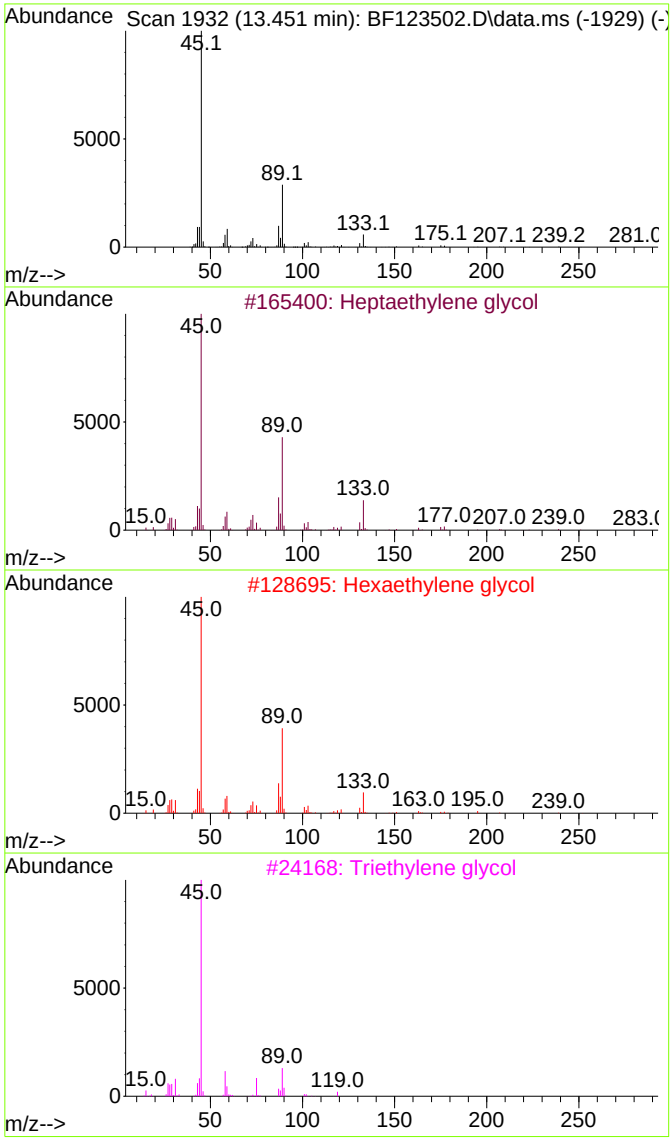
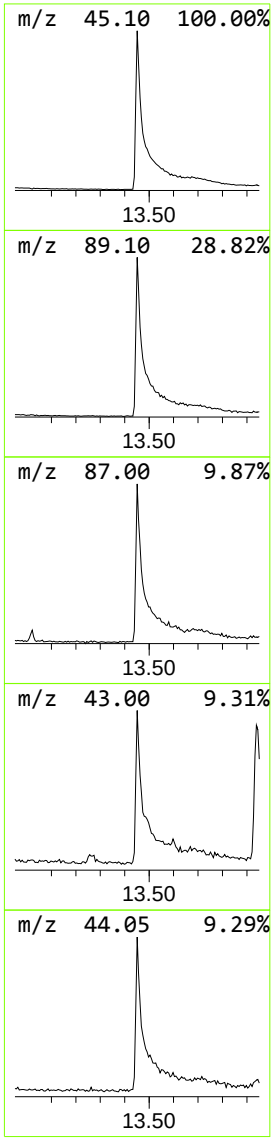
Peak Number 9 Heptaethylene glycol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.451	37.23 ng	2843410	Chrysene-d12	14.080

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptaethylene glycol	326	C14H30O8	005617-32-3	90
2	Hexaethylene glycol	282	C12H26O7	002615-15-8	90
3	Triethylene glycol	150	C6H14O4	000112-27-6	78
4	Acetaldehyde, tetramer	176	C8H16O4	000108-62-3	72
5	Pentaethylene glycol	238	C10H22O6	004792-15-8	72





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Data File : BF123502.D
Acq On : 29 Mar 2021 18:43
Operator : JU/CG
Sample : M1813-03
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : VNJ-236

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF032321.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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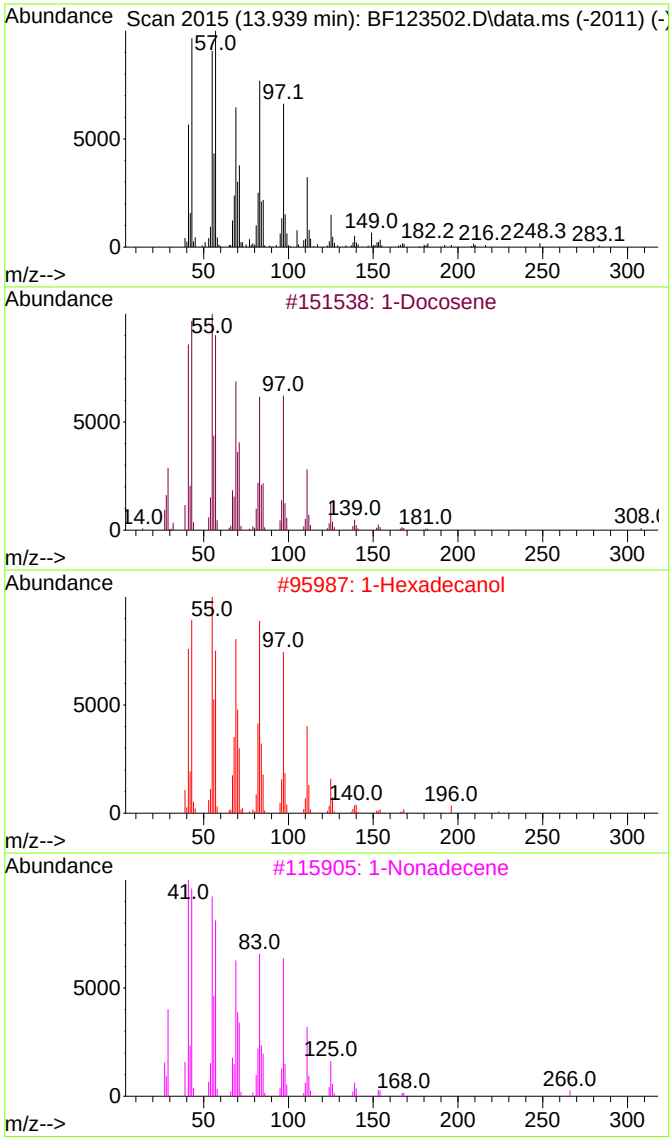
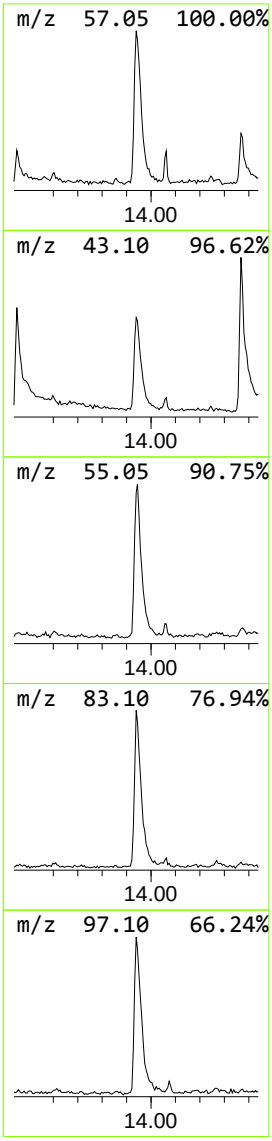
Peak Number 10 1-Docosene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.939	11.91 ng	909492	Chrysene-d12	14.080

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Docosene	308	C22H44	001599-67-3	94
2	1-Hexadecanol	242	C16H34O	036653-82-4	91
3	1-Nonadecene	266	C19H38	018435-45-5	91
4	Acetic acid, chloro-, hexadecyl ...	318	C18H35ClO2	052132-58-8	91
5	Cyclohexadecane	224	C16H32	000295-65-8	91





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Acq On : 29 Mar 2021 18:43
Operator : JU/CG
Sample : M1813-03
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : VNJ-236

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF032321.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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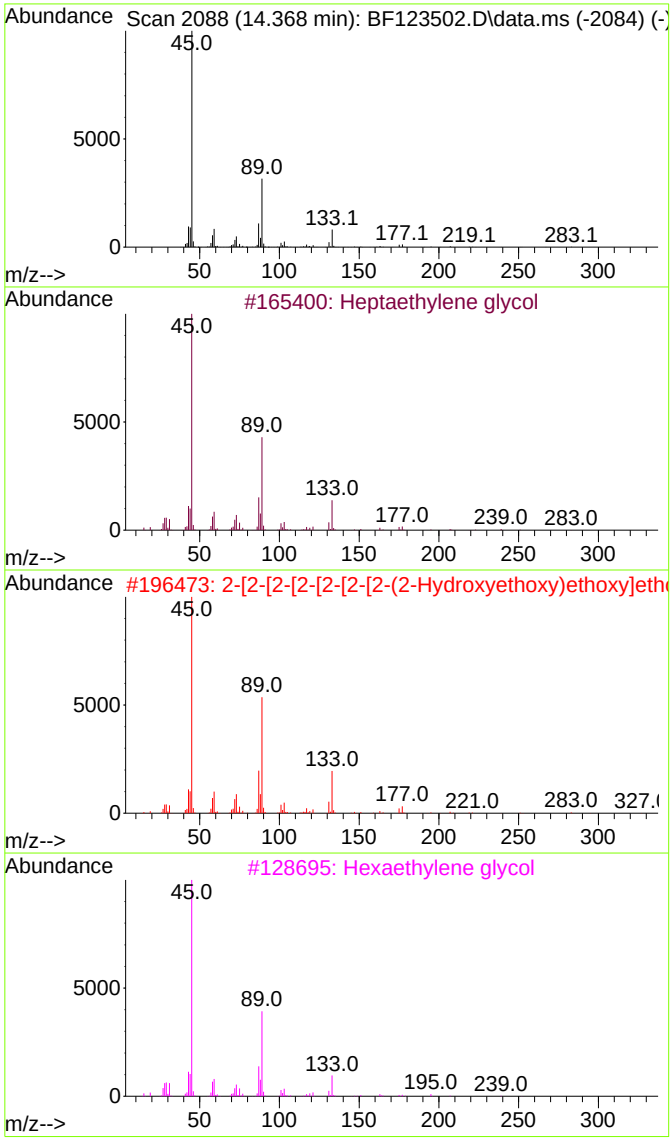
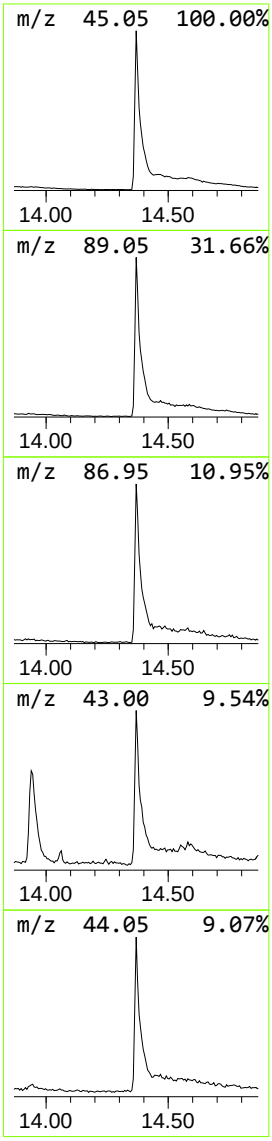
Peak Number 11 Hexaethylene glycol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.368	39.92 ng	3048440	Chrysene-d12	14.080

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptaethylene glycol	326	C14H30O8	005617-32-3	91
2	2-[2-[2-[2-[2-[2-(2-Hydroxyet...	370	C16H34O9	005117-19-1	91
3	Hexaethylene glycol	282	C12H26O7	002615-15-8	83
4	Pentaethylene glycol	238	C10H22O6	004792-15-8	83
5	Triethylene glycol	150	C6H14O4	000112-27-6	72





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Data File : BF123502.D
Acq On : 29 Mar 2021 18:43
Operator : JU/CG
Sample : M1813-03
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
VNJ-236

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF032321.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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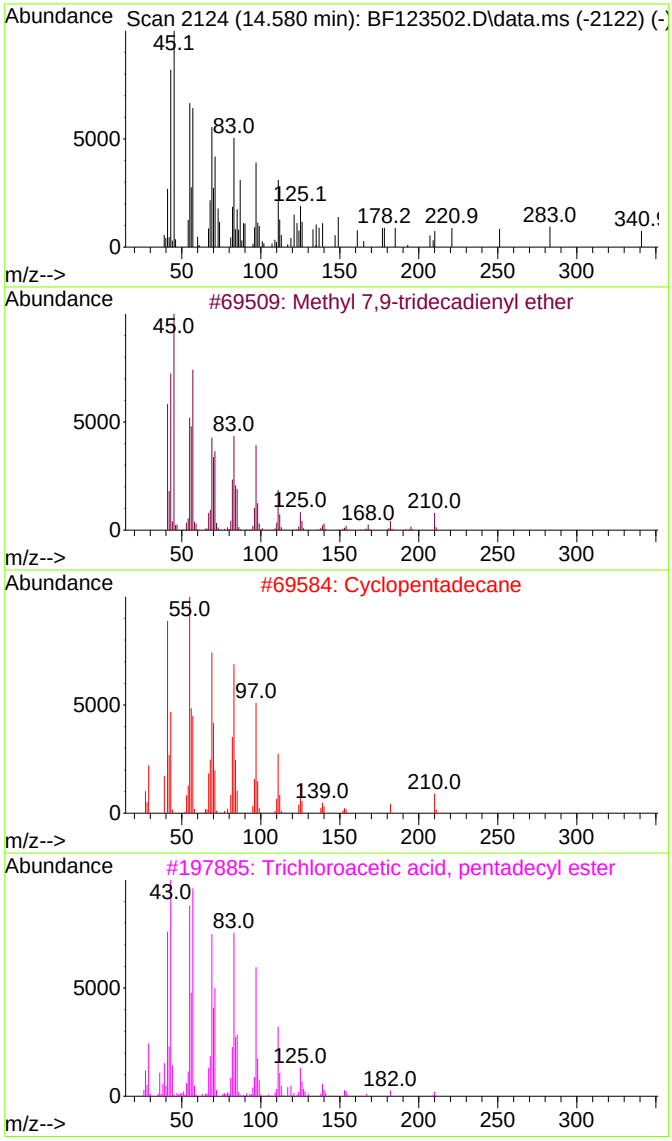
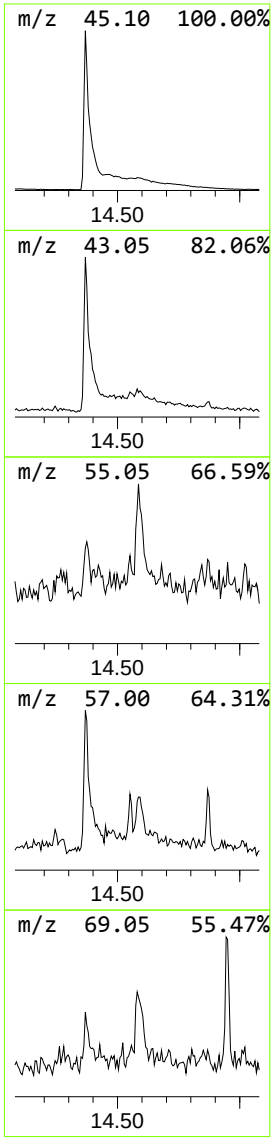
Peak Number 12 Methyl 7,9-tridecadienyl ether Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.580	2.04 ng	155986	Chrysene-d12	14.080

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Methyl 7,9-tridecadienyl ether	210	C14H26O	1000131-00-0	90
2	Cyclopentadecane	210	C15H30	000295-48-7	55
3	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	50
4	Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	46
5	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	46





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Acq On : 29 Mar 2021 18:43
Operator : JU/CG
Sample : M1813-03
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : VNJ-236

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF032321.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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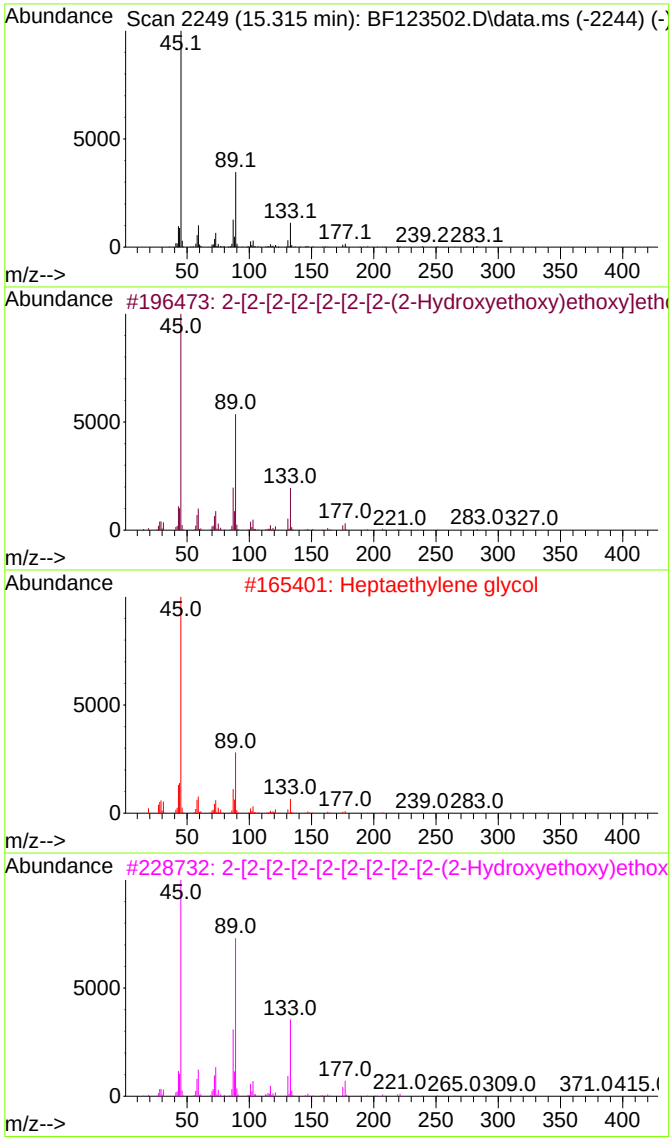
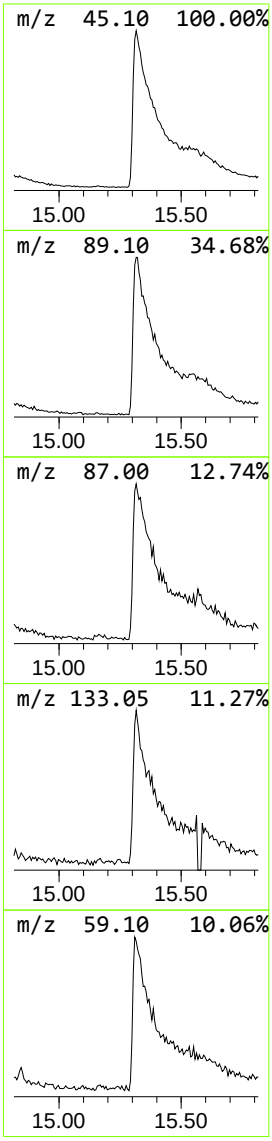
Peak Number 13 Pentaethylene glycol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.315	39.55 ng	2674870	Perylene-d12	15.574

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-[2-[2-[2-[2-[2-[2-(2-Hydroxyet...	370	C16H34O9	005117-19-1	91
2	Heptaethylene glycol	326	C14H30O8	005617-32-3	90
3	2-[2-[2-[2-[2-[2-[2-[2-[2-(2-Hyd...	458	C20H42O11	1000352-12-6	83
4	Pentaethylene glycol	238	C10H22O6	004792-15-8	78
5	2,5,8,11,14-Pentaoxahexadecan-16-ol	252	C11H24O6	023778-52-1	72





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Acq On : 29 Mar 2021 18:43
Operator : JU/CG
Sample : M1813-03
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
VNJ-236

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF032321.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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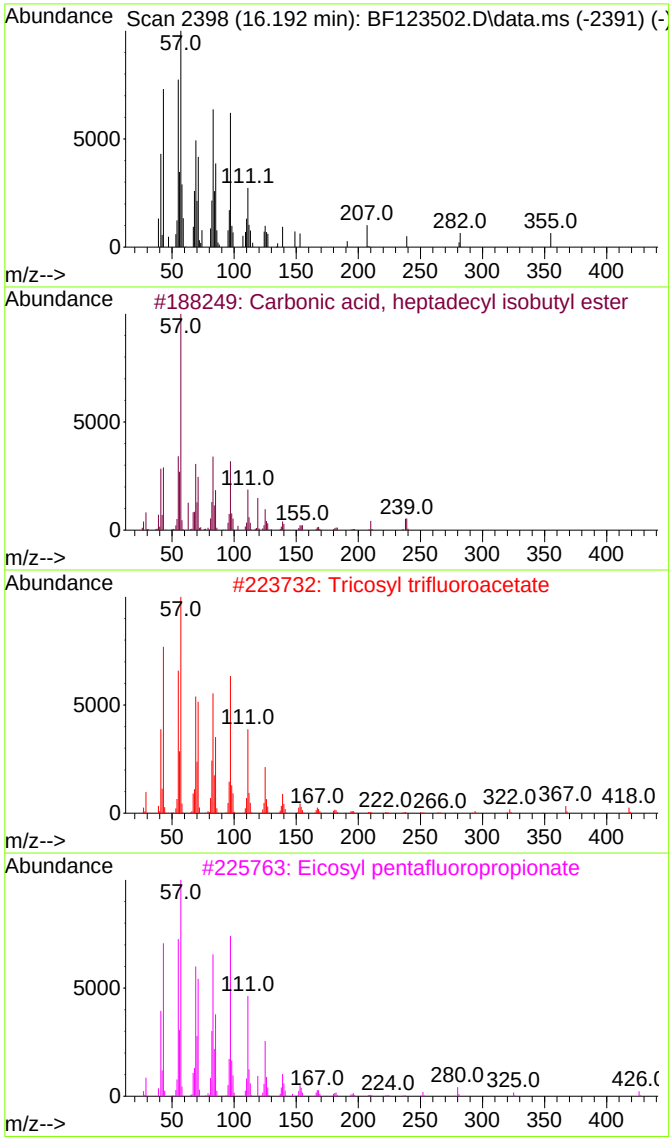
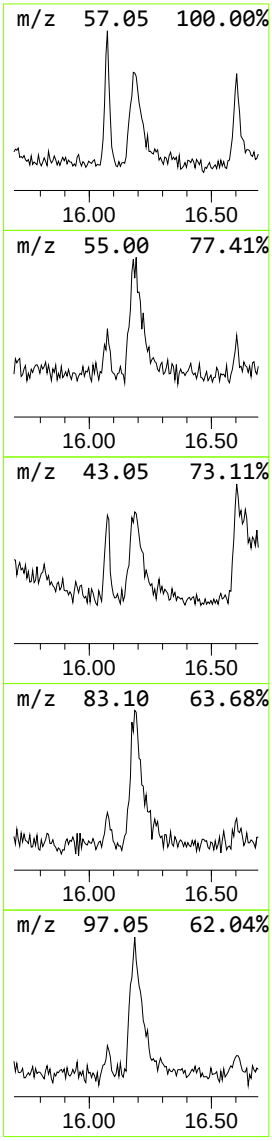
Peak Number 14 Carbonic acid, heptadecyl i... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.192	3.17 ng	214120	Perylene-d12	15.574

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Carbonic acid, heptadecyl isobut...	356	C22H44O3	1000314-61-4	72
2	Tricosyl trifluoroacetate	436	C25H47F3O2	1000351-75-1	68
3	Eicosyl pentafluoropropionate	444	C23H41F5O2	1000351-80-8	64
4	Triacontyl pentafluoropropionate	584	C33H61F5O2	1000351-80-0	64
5	Docosyl pentafluoropropionate	472	C25H45F5O2	1000351-80-9	64





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF032921\
Data File : BF123502.D
Acq On : 29 Mar 2021 18:43
Operator : JU/CG
Sample : M1813-03
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
VNJ-236

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF032321.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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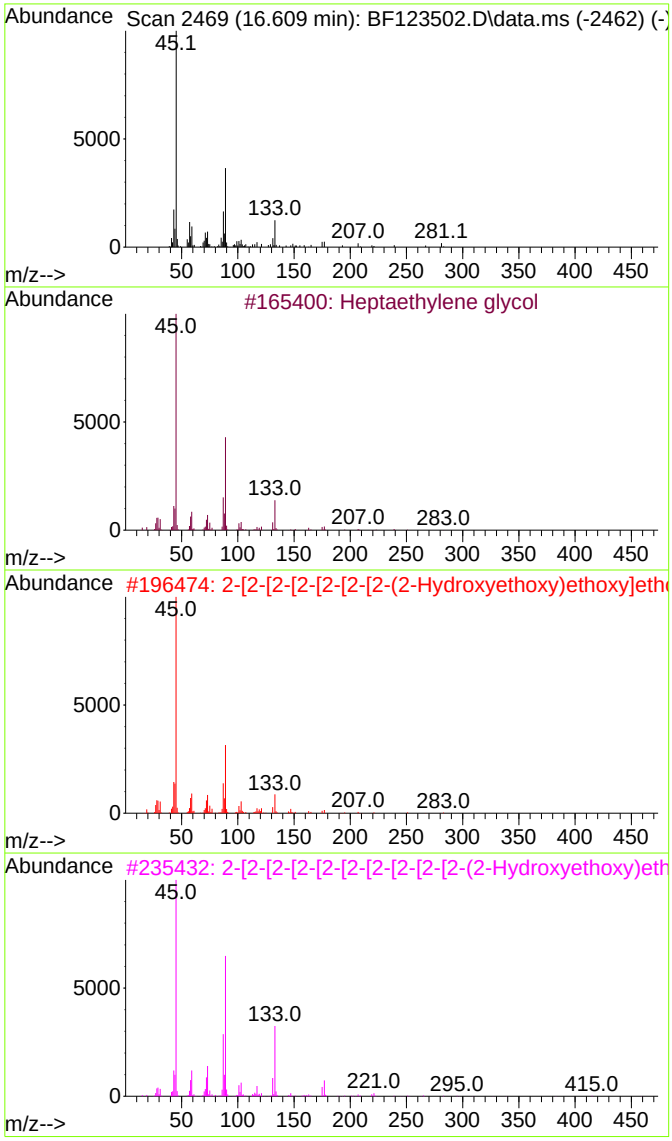
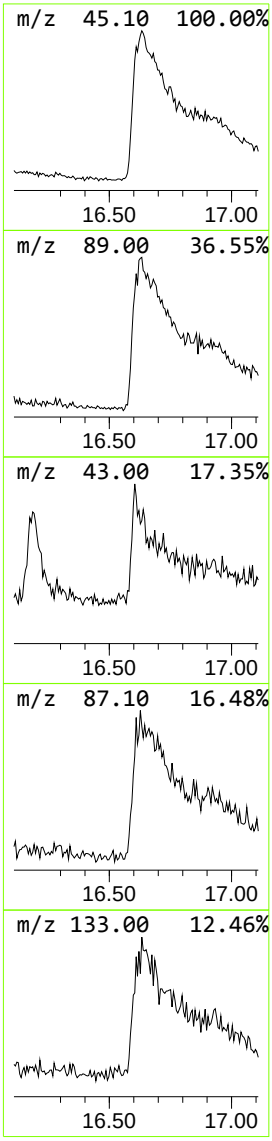
Peak Number 15 unknown16.609 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.609	4.74 ng	320877	Perylene-d12	15.574

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptaethylene glycol	326	C14H30O8	005617-32-3	91
2	2-[2-[2-[2-[2-[2-(2-Hydroxyet...	370	C16H34O9	005117-19-1	91
3	2-[2-[2-[2-[2-[2-[2-[2-[2-(2-...	502	C22H46O12	1000352-13-2	90
4	Hexaethylene glycol	282	C12H26O7	002615-15-8	86
5	2-[2-[2-[2-[2-[2-[2-[2-[2-[2-...	546	C24H50O13	1000352-12-7	86





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF032921\
Data File : BF123502.D
Acq On : 29 Mar 2021 18:43
Operator : JU/CG
Sample : M1813-03
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : VNJ-236

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF032321.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
Butane, 2-metho...	2.240	19.1	ng	1562720	1	6.898	1636880	20.0
Propane, 1,1-di...	2.346	3.0	ng	244787	1	6.898	1636880	20.0
(S)-(+)-1,2-Pro...	3.628	112.0	ng	9169920	1	6.898	1636880	20.0
Propane, 2-meth...	5.122	3.7	ng	302280	1	6.898	1636880	20.0
3-(2-Hydroxyeth...	9.416	12.2	ng	1549640	3	9.939	2538580	20.0
2-[2-[2-[2-[2-[...	11.245	3.0	ng	346578	4	11.433	2326920	20.0
n-Hexadecanoic ...	11.957	6.2	ng	717675	4	11.433	2326920	20.0
Triethylene glycol	12.422	16.1	ng	1874760	4	11.433	2326920	20.0
Heptaethylene g...	13.451	37.2	ng	2843410	5	14.080	1527380	20.0
1-Docosene	13.939	11.9	ng	909492	5	14.080	1527380	20.0
Hexaethylene gl...	14.368	39.9	ng	3048440	5	14.080	1527380	20.0
Methyl 7,9-trid...	14.580	2.0	ng	155986	5	14.080	1527380	20.0
Pentaethylene g...	15.315	39.5	ng	2674870	6	15.574	1352660	20.0
Carbonic acid, ...	16.192	3.2	ng	214120	6	15.574	1352660	20.0
unknown16.609	16.609	4.7	ng	320877	6	15.574	1352660	20.0