LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP061221\
Data File : BP005890.D
Acq On : 12 Jun 2021 15:57
Operator : CG/JU
Sample : M2644-09
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : 1847

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_P\Methods\8270E-BP060821.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP005890.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.858	463	471	483	rBV	647138	1452032	1.01%	0.664%
2	6.240	487	536	537	rBV	14247192	143068134	100.00%	65.444%
3	9.110	987	1024	1029	rBV2	2027791	11282420	7.89%	5.161%
4	10.216	1191	1212	1220	rBV2	407434	1578969	1.10%	0.722%
5	11.151	1360	1371	1380	rBV	1383451	3374060	2.36%	1.543%
6	13.198	1713	1719	1729	rBV2	2187946	4105832	2.87%	1.878%
7	14.592	1948	1956	1963	rVB3	1655020	4290324	3.00%	1.963%
8	15.210	2057	2061	2067	rVB	1857915	2613131	1.83%	1.195%
9	16.057	2201	2205	2209	rBV	1533732	2073071	1.45%	0.948%
10	16.104	2209	2213	2218	rVV2	1551549	2105273	1.47%	0.963%
11	16.351	2252	2255	2260	rVB	1156019	1571588	1.10%	0.719%
12	17.133	2384	2388	2393	rVB	1310262	1750912	1.22%	0.801%
13	18.157	2559	2562	2567	rVB	2256179	2905118	2.03%	1.329%
14	19.763	2832	2835	2840	rVB	3898501	4502137	3.15%	2.059%
15	19.869	2849	2853	2858	rVB	3616875	4518876	3.16%	2.067%
16	21.074	3053	3058	3070	rVB	4951884	7254657	5.07%	3.319%
17	22.321	3265	3270	3284	rVB	4616067	6730254	4.70%	3.079%
18	23.951	3541	3547	3553	rBV	2155329	4135956	2.89%	1.892%
19	25.004	3721	3726	3737	rVB2	1273295	3635997	2.54%	1.663%
20	25.757	3848	3854	3865	rVB	2059351	5663491	3.96%	2.591%

Sum of corrected areas: 218612232

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP061221\
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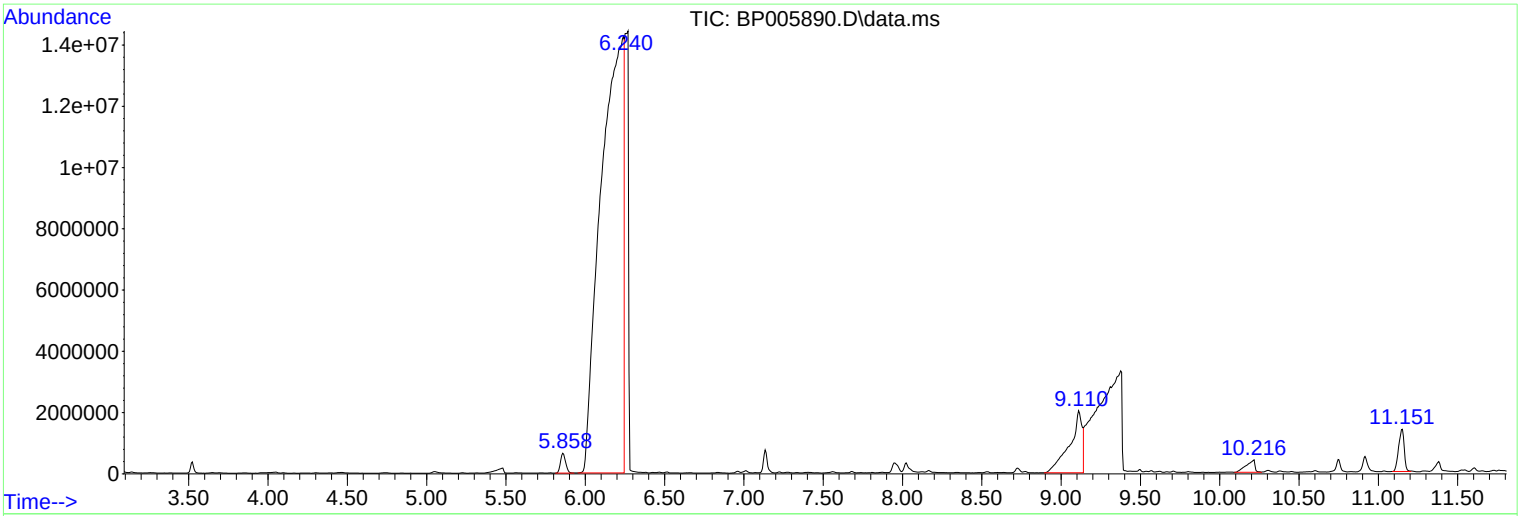
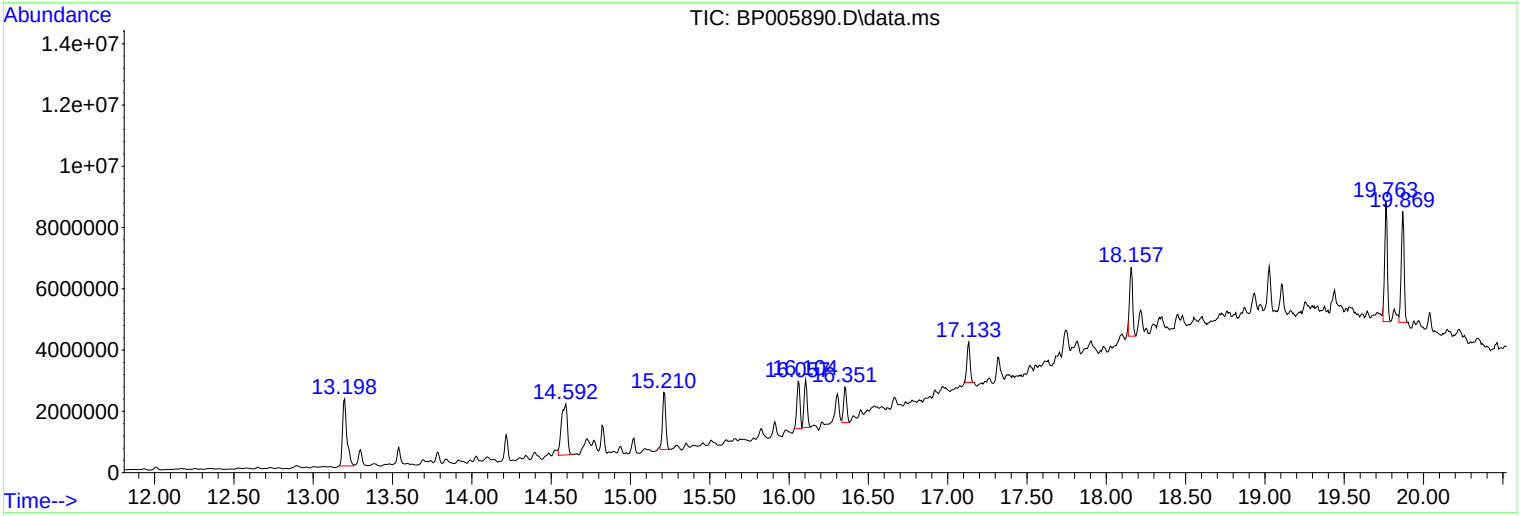
Sample : M2644-09
Misc :
ALS Vial : 7 Sample Multiplier: 1

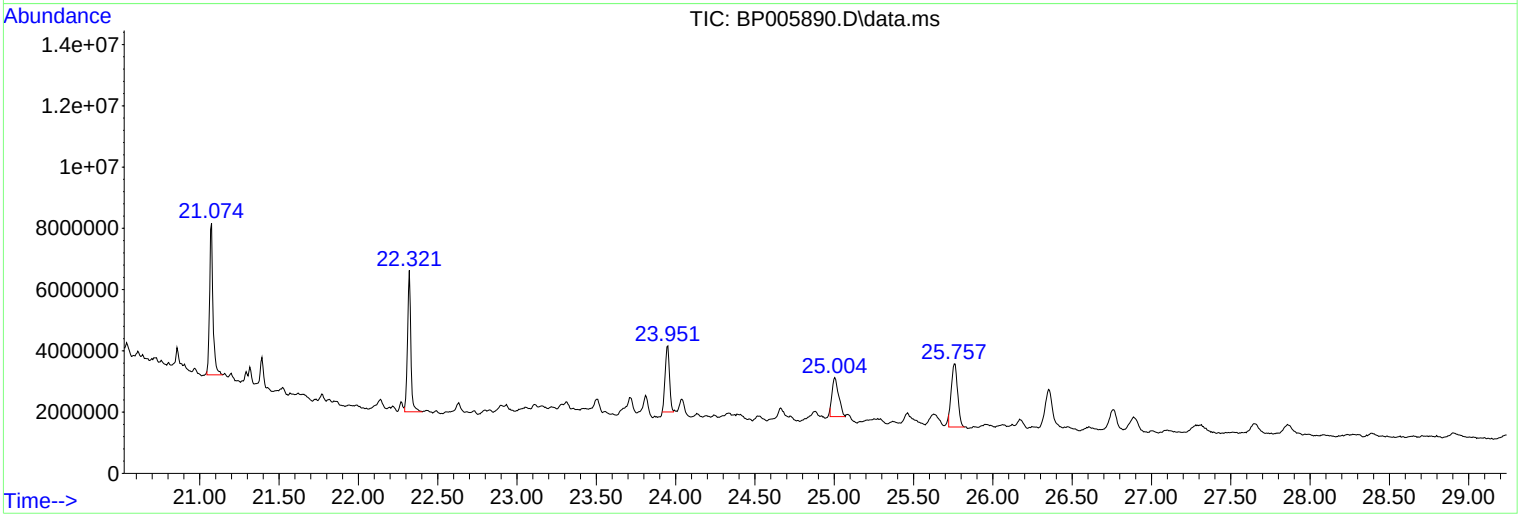
Instrument :
BNA_P
ClientSampleId :
1847

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP060821.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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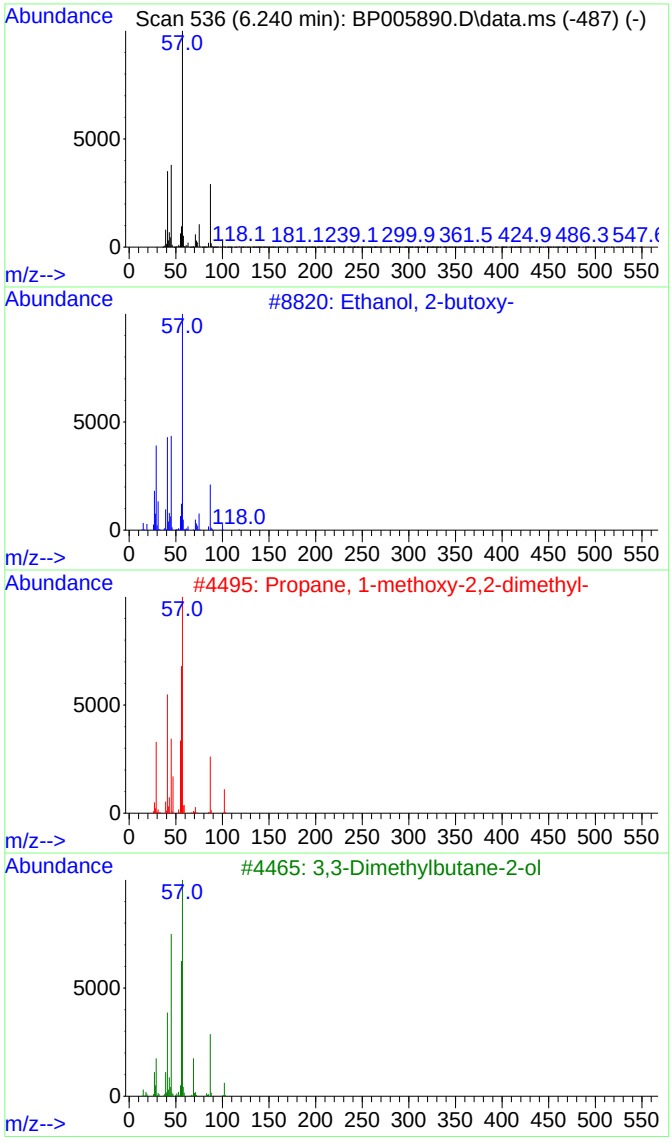
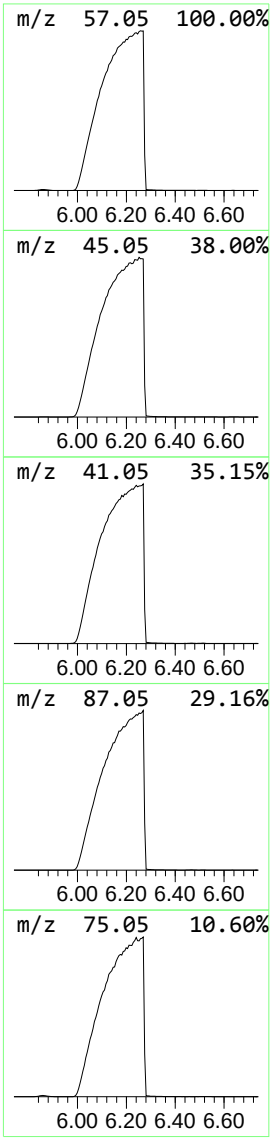
Peak Number 1 Ethanol, 2-butoxy- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.240	253.61 ng	143068000	1,4-Dichlorobenzene-d4	7.946

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-butoxy-	118	C6H14O2	000111-76-2	90
2	Propane, 1-methoxy-2,2-dimethyl-	102	C6H14O	001118-00-9	40
3	3,3-Dimethylbutane-2-ol	102	C6H14O	000464-07-3	37
4	Formic acid, 3,3-dimethylbut-2-y...	130	C7H14O2	1000368-20-5	36
5	Butane, 1-(1-methylpropoxy)-	130	C8H18O	000999-65-5	25





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Operator : CG/JU
Sample : M2644-09
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : 1847

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP060821.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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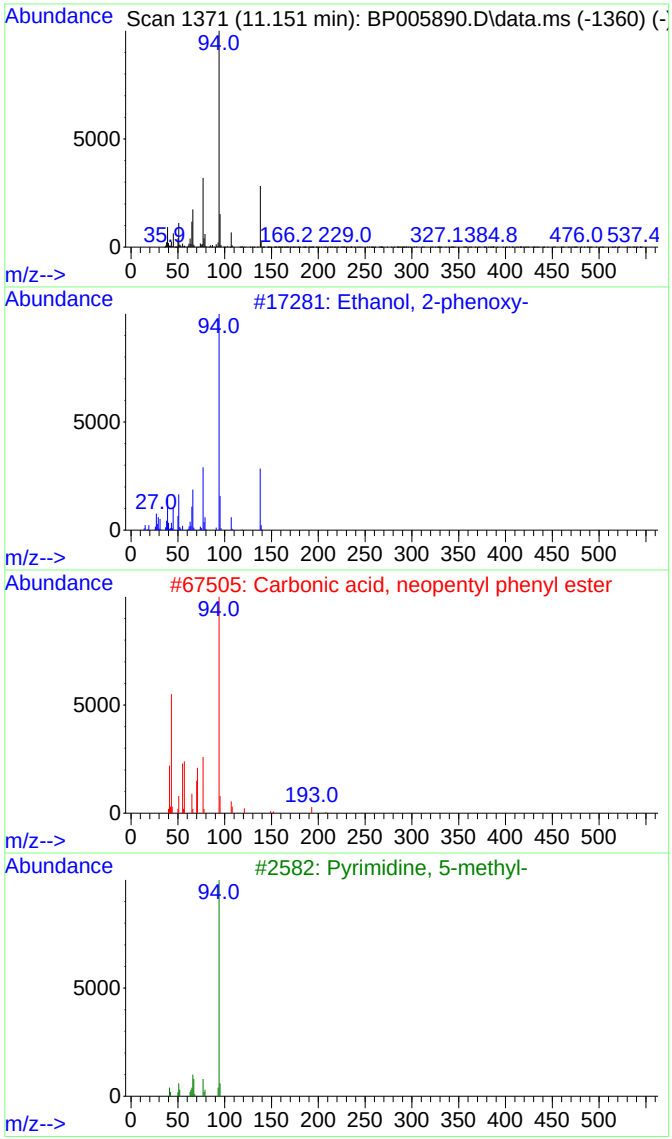
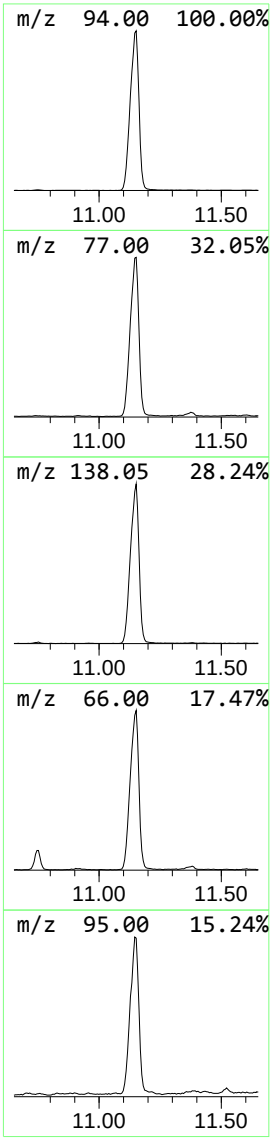
Peak Number 2 Ethanol, 2-phenoxy- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.151	20.00 ng	3374060	Naphthalene-d8	10.746

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-phenoxy-	138	C8H10O2	000122-99-6	95
2	Carbonic acid, neopentyl phenyl ...	208	C12H16O3	013183-19-2	64
3	Pyrimidine, 5-methyl-	94	C5H6N2	002036-41-1	59
4	Benzene, ethoxy-	122	C8H10O	000103-73-1	53
5	2-Pyridinecarboxylic acid, 3-amino-	138	C6H6N2O2	001462-86-8	53





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Sample : M2644-09
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : 1847

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP060821.M
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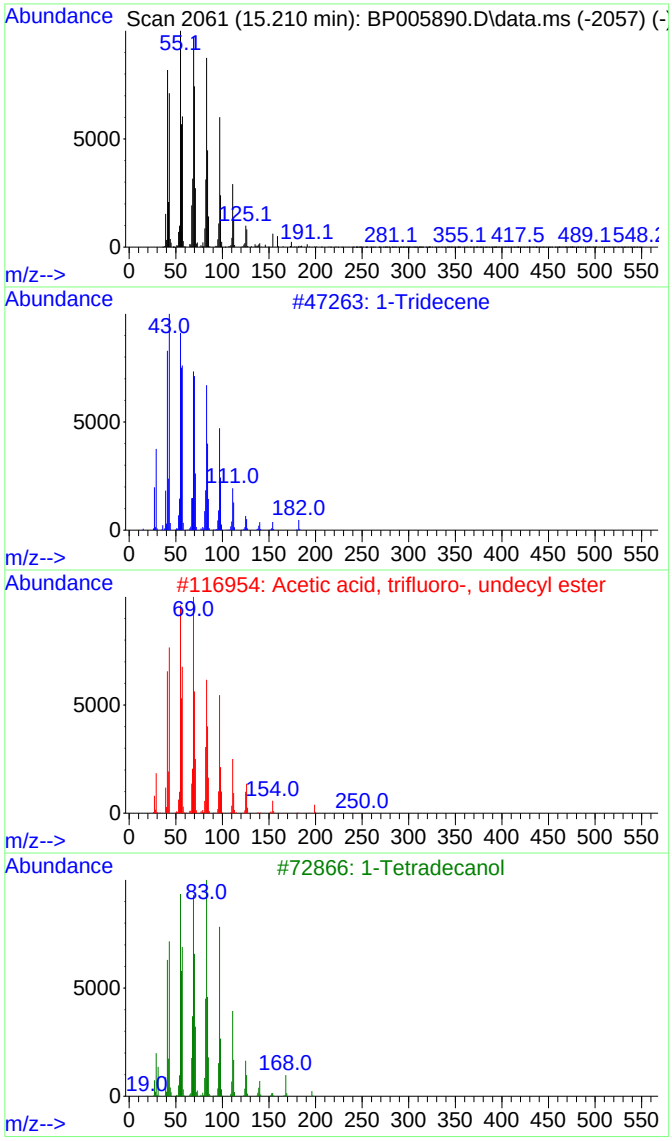
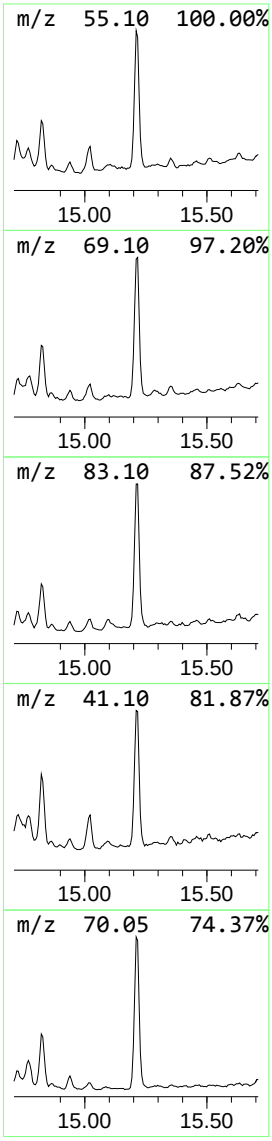
Peak Number 3 1-Tridecene Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.210	12.18 ng	2613130	Acenaphthene-d10	14.569

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Tridecene	182	C13H26	002437-56-1	95
2	Acetic acid, trifluoro-, undecyl...	268	C13H23F3O2	053800-01-4	91
3	1-Tetradecanol	214	C14H30O	000112-72-1	91
4	n-Tridecan-1-ol	200	C13H28O	000112-70-9	91
5	5-Tetradecene, (E)-	196	C14H28	041446-66-6	91





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Sample : M2644-09
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Instrument : BNA_P
ClientSampleId : 1847

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP060821.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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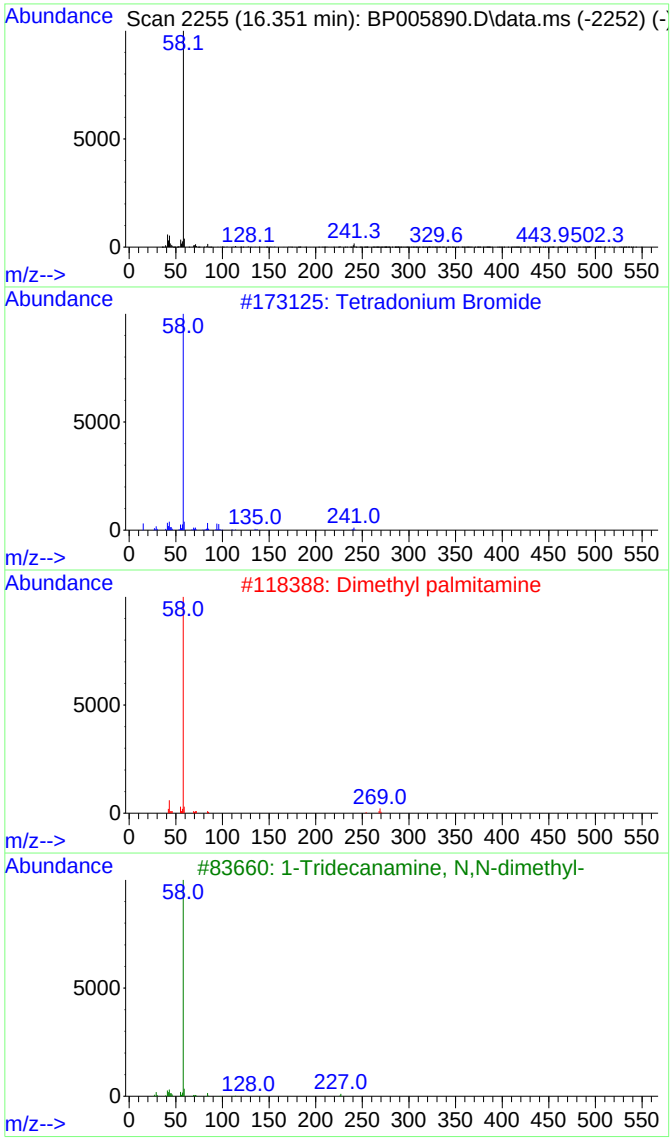
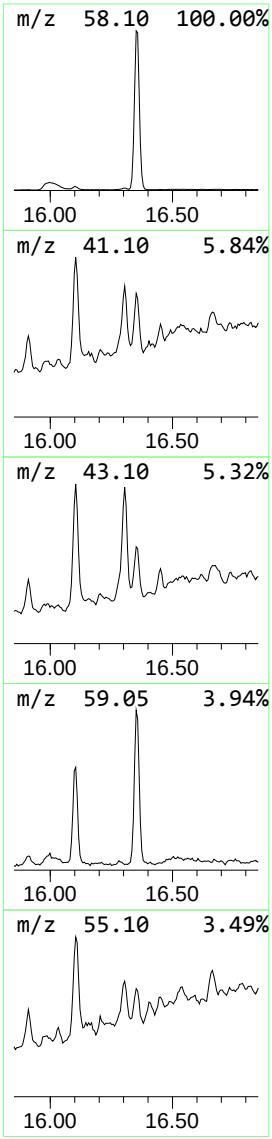
Peak Number 4 Tetradonium Bromide Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.351	17.95 ng	1571590	Phenanthrene-d10	17.316

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetradonium Bromide	335	C17H38BrN	001119-97-7	78
2	Dimethyl palmitamine	269	C18H39N	000112-69-6	72
3	1-Tridecanamine, N,N-dimethyl-	227	C15H33N	017373-29-4	72
4	Cetrimonium Bromide	363	C19H42BrN	000057-09-0	72
5	1-Dodecanamine, N,N-dimethyl-	213	C14H31N	000112-18-5	64





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Data File : BP005890.D
Acq On : 12 Jun 2021 15:57
Operator : CG/JU
Sample : M2644-09
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : 1847

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP060821.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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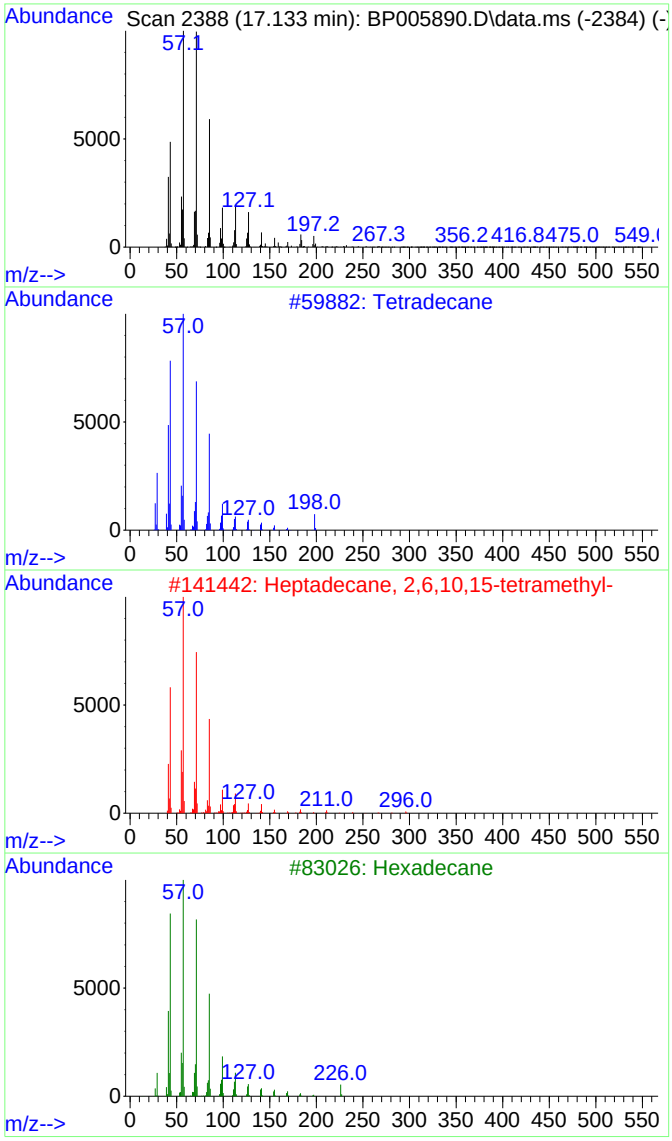
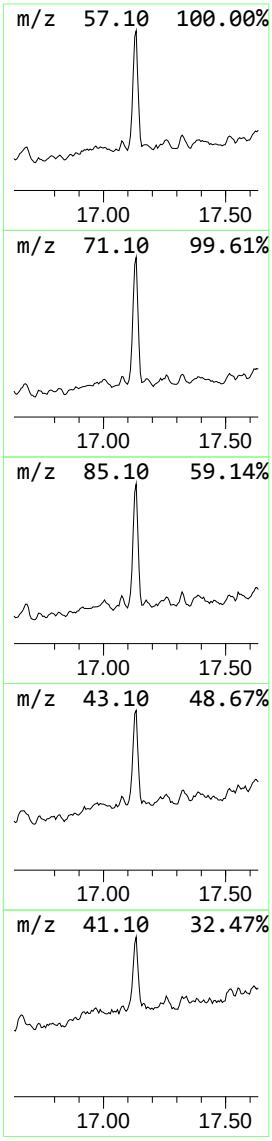
Peak Number 5 Tetradecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.133	20.00 ng	1750910	Phenanthrene-d10	17.316

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetradecane	198	C14H30	000629-59-4	90
2	Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	86
3	Hexadecane	226	C16H34	000544-76-3	80
4	Pentadecane, 2,6,10-trimethyl-	254	C18H38	003892-00-0	74
5	Hexadecane, 2,6,10,14-tetramethyl-	282	C20H42	000638-36-8	74





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Sample : M2644-09
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : 1847

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP060821.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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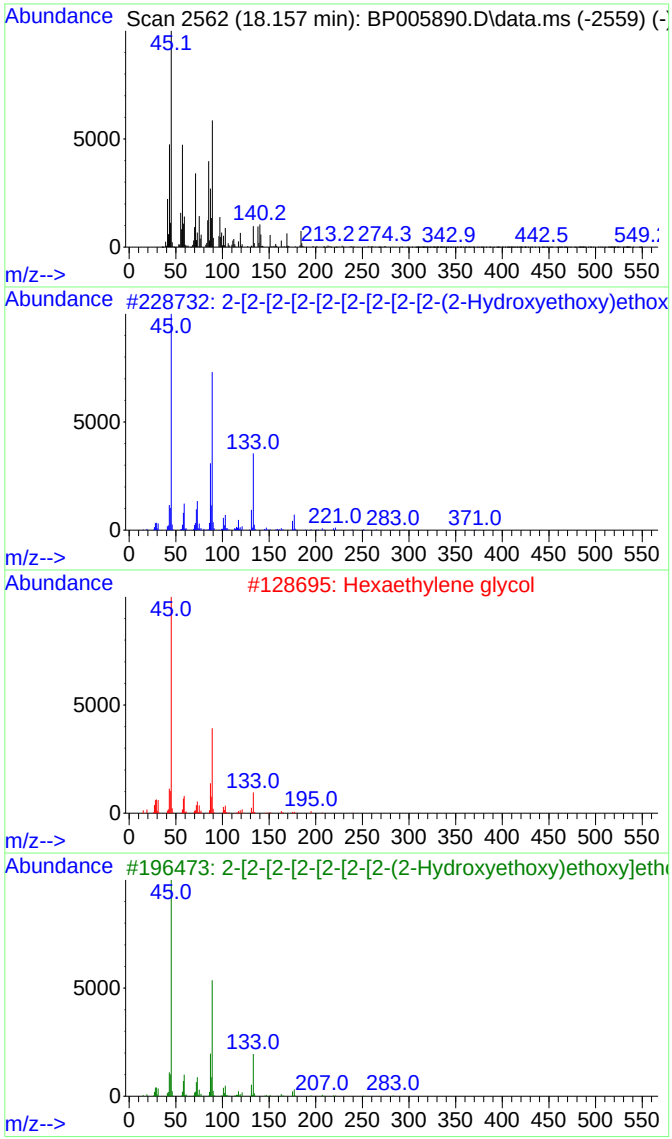
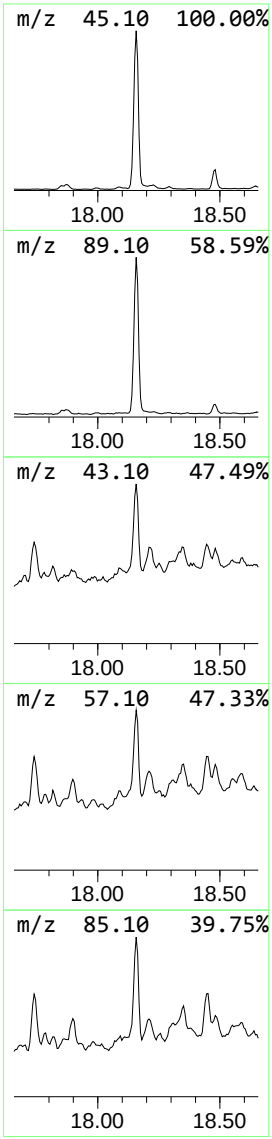
Peak Number 6 2-[2-[2-[2-[2-[2-[2-[2-[2-(... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.157	33.18 ng	2905120	Phenanthrene-d10	17.316

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	50
2	Hexaethylene glycol	282	C12H26O7	002615-15-8	50
3	2-[2-[2-[2-[2-[2-[2-(2-Hydroxyet...	370	C16H34O9	005117-19-1	49
4	2-[2-[2-[2-[2-[2-[2-[2-[2-[2-(2-...	502	C22H46O12	1000352-13-2	49
5	2-[2-[2-[2-[2-[2-[2-[2-(2-Hydrox...	414	C18H38O10	1000352-12-5	49





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Instrument : BNA_P
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TIC Library : C:\DATABASE\NIST11.L
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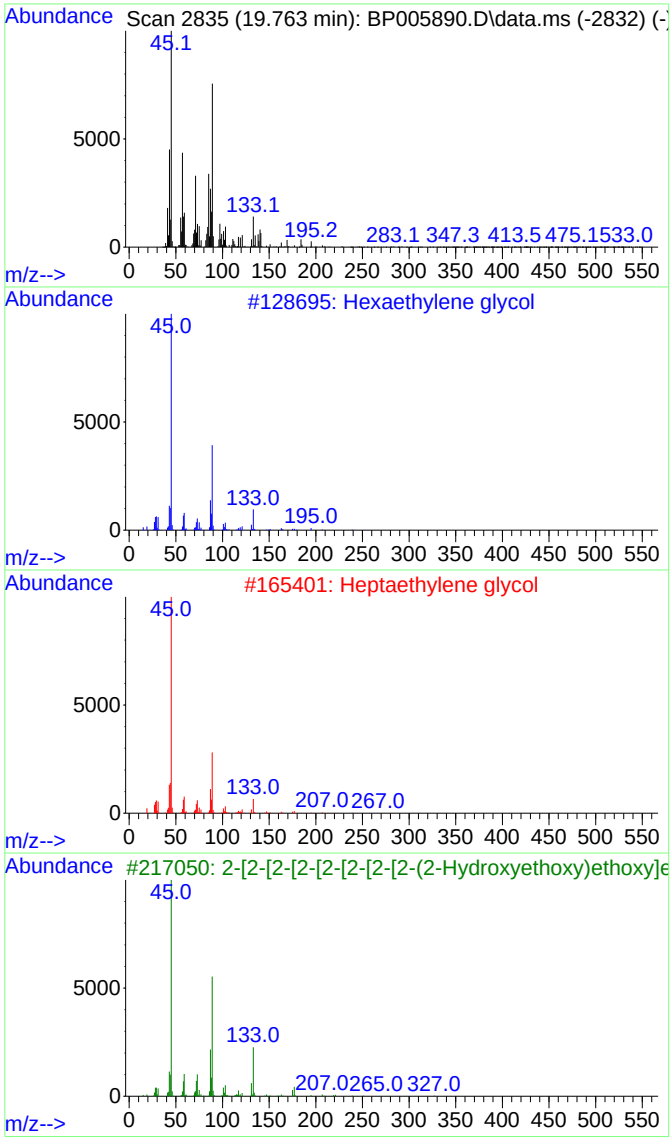
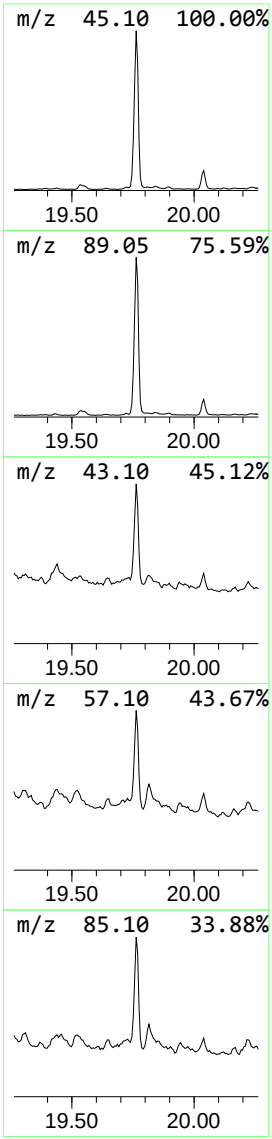
Peak Number 7 Hexaethylene glycol Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.763	12.41 ng	4502140	Chrysene-d12	21.392

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexaethylene glycol	282	C12H26O7	002615-15-8	90
2	Heptaethylene glycol	326	C14H30O8	005617-32-3	87
3	2-[2-[2-[2-[2-[2-[2-(2-Hydrox...	414	C18H38O10	1000352-12-5	86
4	Pentaethylene glycol	238	C10H22O6	004792-15-8	86
5	2-[2-[2-[2-[2-[2-(2-Hydroxyet...	370	C16H34O9	005117-19-1	72





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TIC Library : C:\DATABASE\NIST11.L
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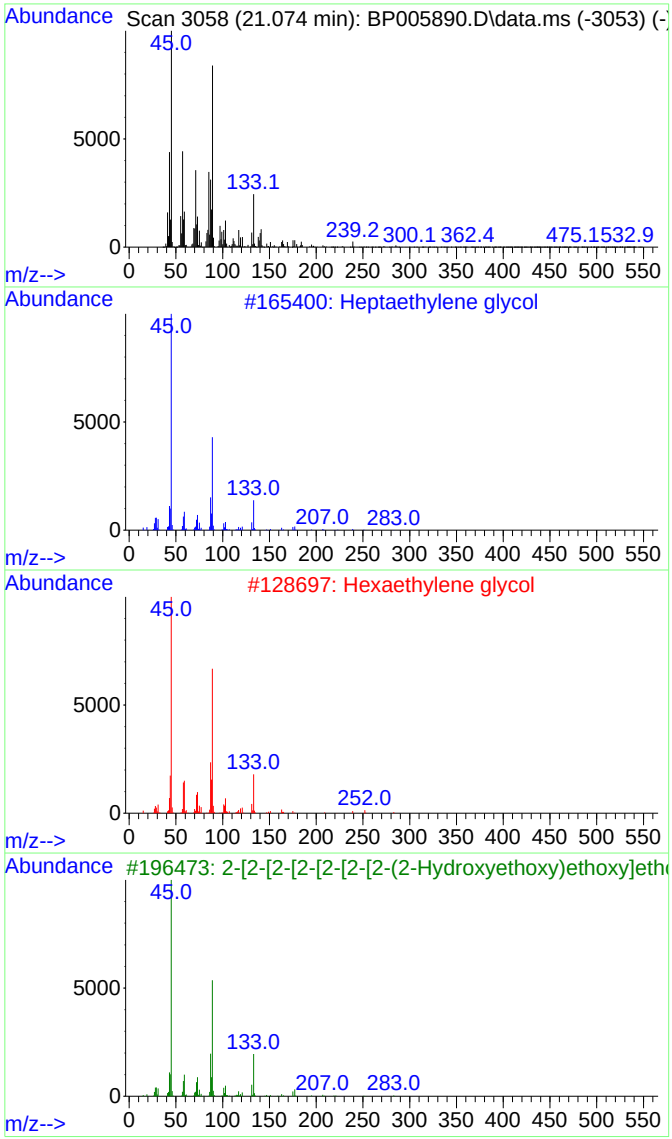
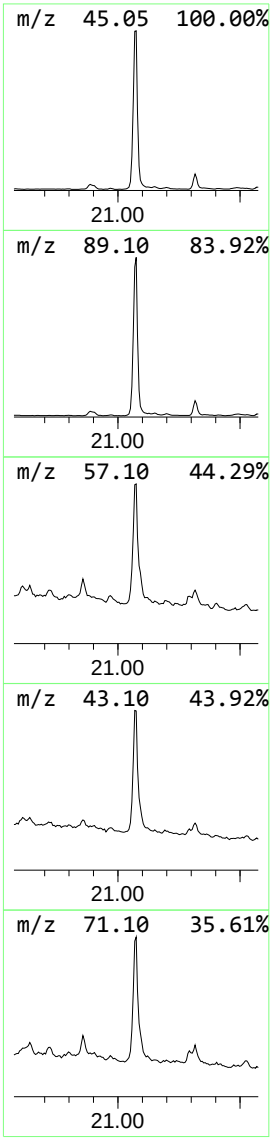
Peak Number 8 Heptaethylene glycol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.074	20.00 ng	7254660	Chrysene-d12	21.392

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptaethylene glycol	326	C14H30O8	005617-32-3	91
2	Hexaethylene glycol	282	C12H26O7	002615-15-8	91
3	2-[2-[2-[2-[2-[2-(2-Hydroxyet...	370	C16H34O9	005117-19-1	91
4	2-[2-[2-[2-[2-[2-[2-(2-Hydrox...	414	C18H38O10	1000352-12-5	91
5	2-[2-[2-[2-[2-[2-[2-[2-(2-Hyd...	458	C20H42O11	1000352-12-6	90





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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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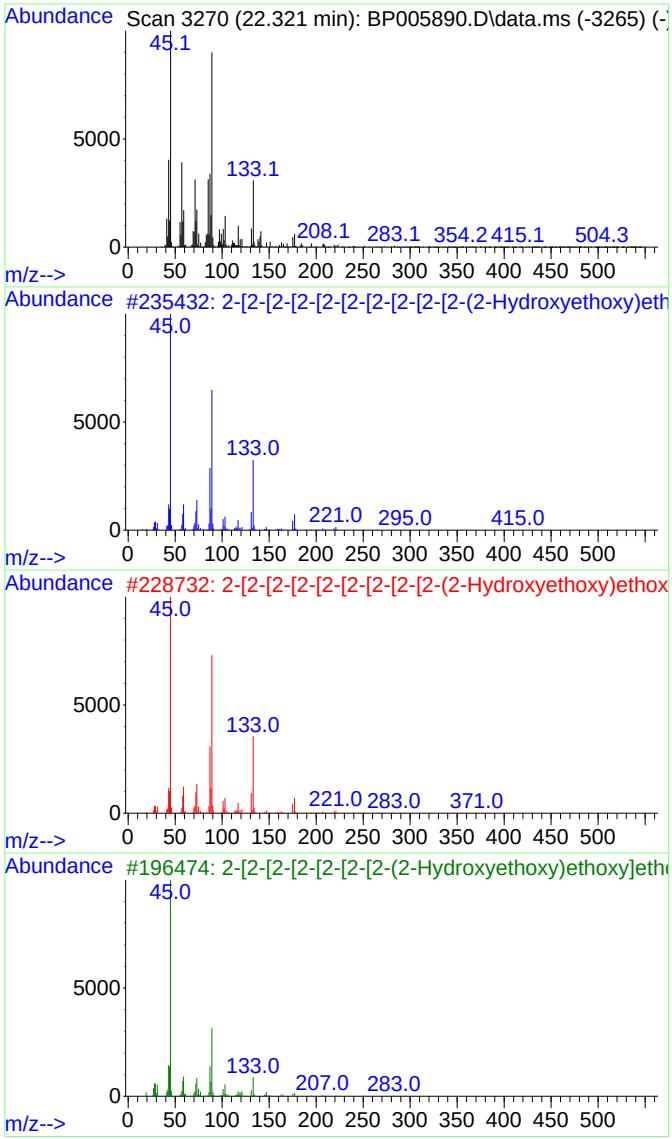
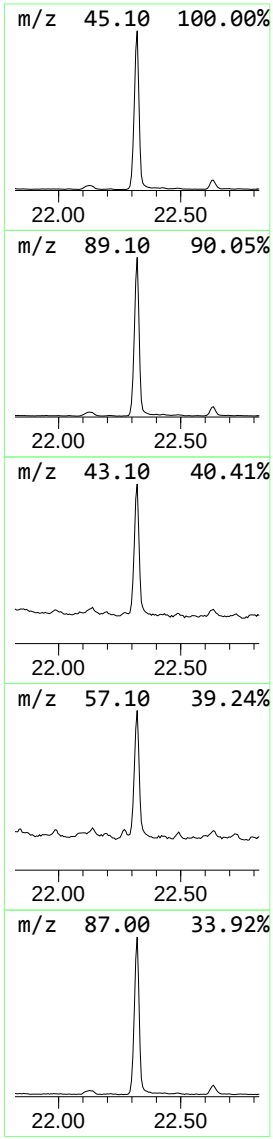
Peak Number 9 2-[2-[2-[2-[2-[2-[2-[2-[2-[... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.321	18.55 ng	6730250	Chrysene-d12	21.392

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-[2-[2-[2-[2-[2-[2-[2-[2-[2-(2-...	502	C22H46O12	1000352-13-2	91
2	2-[2-[2-[2-[2-[2-[2-[2-[2-(2-Hyd...	458	C20H42O11	1000352-12-6	91
3	2-[2-[2-[2-[2-[2-[2-(2-Hydroxyet...	370	C16H34O9	005117-19-1	91
4	2-[2-[2-[2-[2-[2-[2-[2-(2-Hydrox...	414	C18H38O10	1000352-12-5	91
5	Hexaethylene glycol	282	C12H26O7	002615-15-8	91





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Instrument : BNA_P
ClientSampleId : 1847

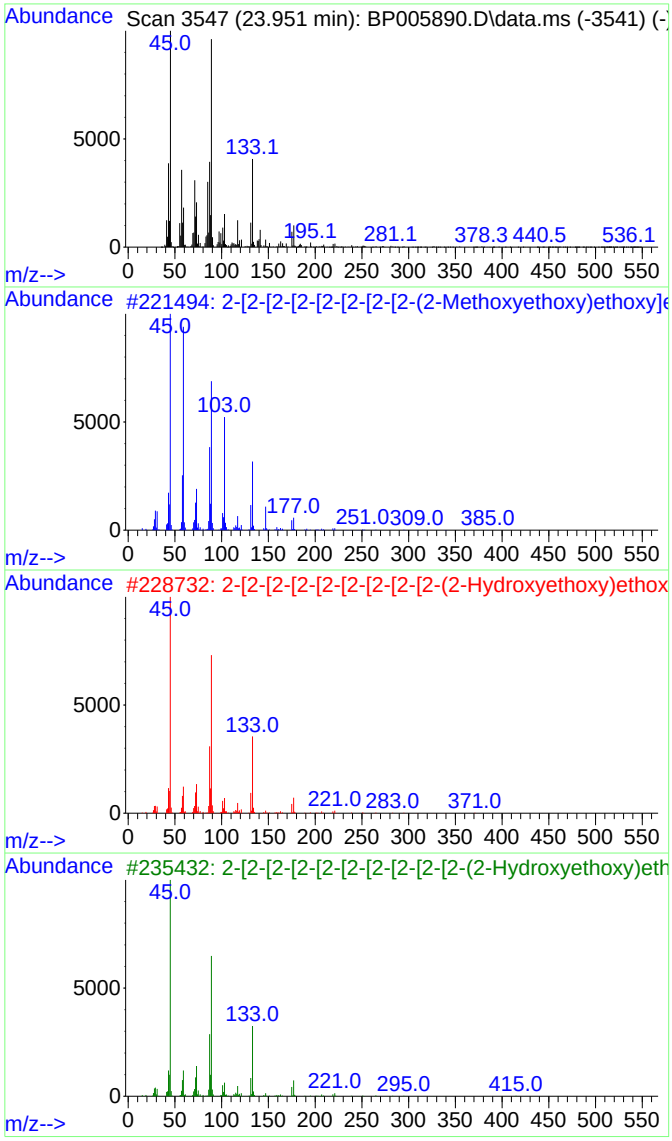
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP060821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

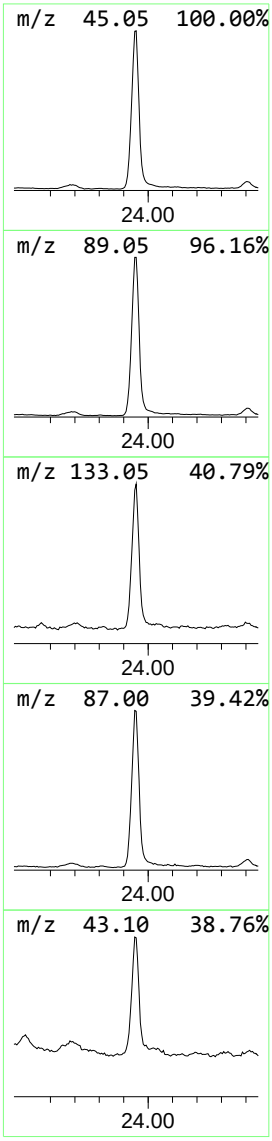
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 2-[2-[2-[2-[2-[2-[2-[2-(2-M... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.951	20.00 ng	4135960	Perylene-d12	23.810

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-[2-[2-[2-[2-[2-[2-[2-(2-Methox...	428	C19H40O10	1000352-04-3	91
2	2-[2-[2-[2-[2-[2-[2-[2-[2-(2-Hyd...	458	C20H42O11	1000352-12-6	90
3	2-[2-[2-[2-[2-[2-[2-[2-[2-[2-(2-...	502	C22H46O12	1000352-13-2	87
4	Heptaethylene glycol monododecyl...	494	C26H54O8	003055-97-8	83
5	Hexaethylene glycol monododecyl ...	450	C24H50O7	003055-96-7	83





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP061221\
Data File : BP005890.D
Acq On : 12 Jun 2021 15:57
Operator : CG/JU
Sample : M2644-09
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : 1847

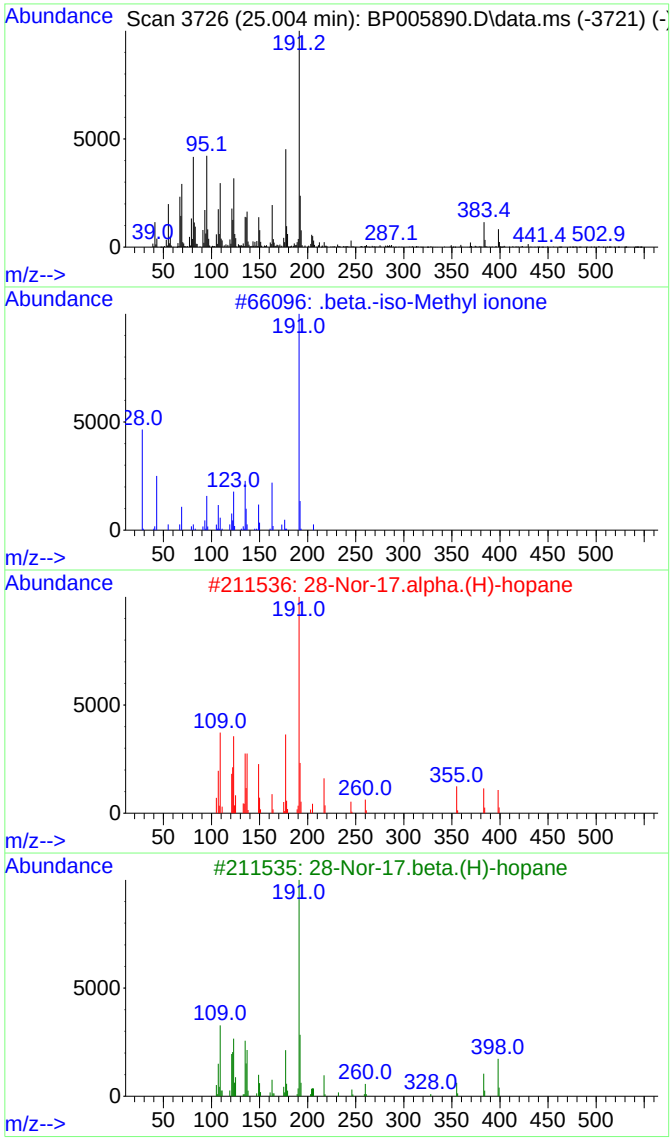
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP060821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

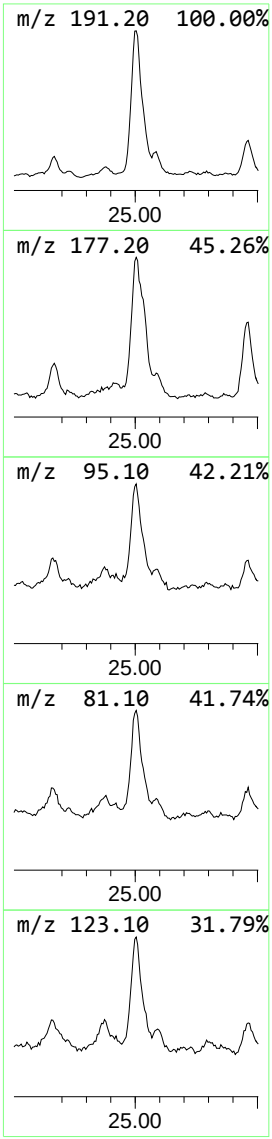
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 11 .beta.-iso-Methyl ionone Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
25.004	17.58 ng	3636000	Perylene-d12	23.810

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	.beta.-iso-Methyl ionone	206	C14H22O	1000285-40-2	52
2	28-Nor-17.alpha.(H)-hopane	398	C29H50	053584-60-4	42
3	28-Nor-17.beta.(H)-hopane	398	C29H50	036728-72-0	35
4	3-Fluoro-4-trifluoromethylbenzoi...	380	C15H6Cl2F4O3	1000357-35-8	30
5	Acetamide, N-[3-[[(2,5-dioxo-1-p...	303	C16H21N3O3	027550-64-7	27





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP061221\
Data File : BP005890.D
Acq On : 12 Jun 2021 15:57
Operator : CG/JU
Sample : M2644-09
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : 1847

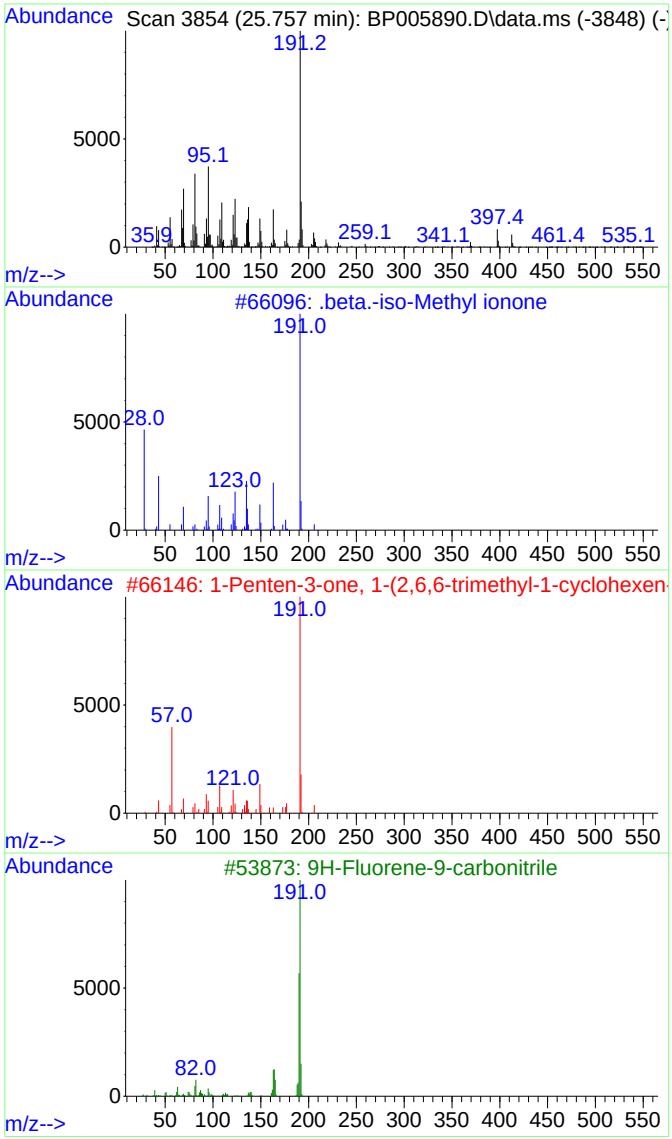
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP060821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

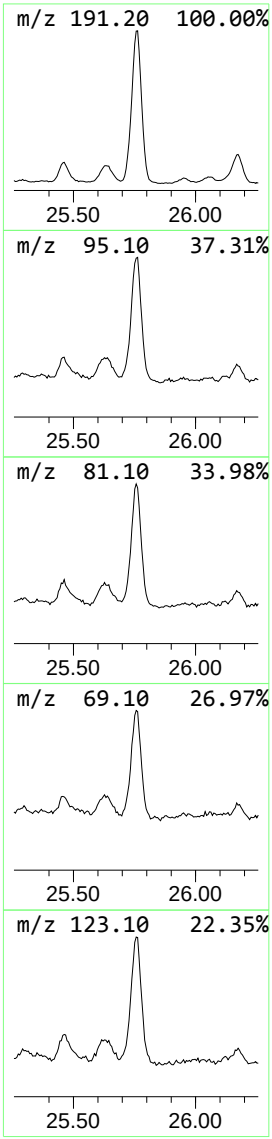
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 12 1-Penten-3-one, 1-(2,6,6-tr... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
25.756	27.39 ng	5663490	Perylene-d12	23.810

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	.beta.-iso-Methyl ionone	206	C14H22O	1000285-40-2	72
2	1-Penten-3-one, 1-(2,6,6-trimeth...	206	C14H22O	000127-43-5	60
3	9H-Fluorene-9-carbonitrile	191	C14H9N	001529-40-4	47
4	1-Cyclohexene, 1,3,3-trimethyl-2...	206	C14H22O	1000197-08-4	40
5	4-Fluoro-3-trifluoromethylbenzoi...	390	C21H30F4O2	1000338-68-0	38





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP061221\
Data File : BP005890.D
Acq On : 12 Jun 2021 15:57
Operator : CG/JU
Sample : M2644-09
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : 1847

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP060821.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
Ethanol, 2-butoxy-	6.240	253.6	ng	143068000	1	7.946	11282400	20.0
Ethanol, 2-phen...	11.151	20.0	ng	3374060	2	10.746	3374060	20.0
1-Tridecene	15.210	12.2	ng	2613130	3	14.569	4290320	20.0
Tetradonium Bro...	16.351	17.9	ng	1571590	4	17.316	1750910	20.0
Tetradecane	17.133	20.0	ng	1750910	4	17.316	1750910	20.0
2-[2-[2-[2-[2-[...	18.157	33.2	ng	2905120	4	17.316	1750910	20.0
Hexaethylene gl...	19.763	12.4	ng	4502140	5	21.392	7254660	20.0
Heptaethylene g...	21.074	20.0	ng	7254660	5	21.392	7254660	20.0
2-[2-[2-[2-[2-[...	22.321	18.6	ng	6730250	5	21.392	7254660	20.0
2-[2-[2-[2-[2-[...	23.951	20.0	ng	4135960	6	23.810	4135960	20.0
.beta.-iso-Meth...	25.004	17.6	ng	3636000	6	23.810	4135960	20.0
1-Penten-3-one,...	25.756	27.4	ng	5663490	6	23.810	4135960	20.0