LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP041321\
Data File : BP005293.D
Acq On : 13 Apr 2021 18:34
Operator : CG/JU
Sample : M1998-06
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : SB-4B

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-BP040921.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP005293.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.816	292	294	302	rVB	112231	165249	6.90%	1.189%
2	5.281	368	373	389	rVB	1064991	1542743	64.40%	11.102%
3	6.828	632	636	637	rBV	43205	50055	2.09%	0.360%
4	6.869	637	643	656	rVB2	1049421	2395419	100.00%	17.238%
5	7.675	774	780	786	rVB	240818	358571	14.97%	2.580%
6	7.740	786	791	800	rVB	89882	136138	5.68%	0.980%
7	8.840	970	978	997	rVB	626313	1039977	43.42%	7.484%
8	10.240	1210	1216	1228	rBV2	59304	150745	6.29%	1.085%
9	10.463	1247	1254	1260	rBV	255236	413646	17.27%	2.977%
10	11.487	1424	1428	1441	rBV8	10430	31314	1.31%	0.225%
11	11.981	1506	1512	1525	rBV	181511	318350	13.29%	2.291%
12	12.951	1667	1677	1687	rBV	1075989	1550358	64.72%	11.157%
13	13.745	1807	1812	1816	rVB4	19247	28151	1.18%	0.203%
14	13.816	1816	1824	1828	rVV3	21913	49226	2.06%	0.354%
15	14.339	1907	1913	1921	rVB2	311154	464572	19.39%	3.343%
16	15.839	2162	2168	2175	rBV	263577	384359	16.05%	2.766%
17	16.086	2203	2210	2214	rBV4	30040	59898	2.50%	0.431%
18	16.869	2339	2343	2348	rBV7	32544	54950	2.29%	0.395%
19	16.916	2348	2351	2358	rVB4	21566	32414	1.35%	0.233%
20	17.104	2377	2383	2387	rBV	327294	470786	19.65%	3.388%
21	17.145	2387	2390	2394	rVB2	22777	29487	1.23%	0.212%
22	17.198	2395	2399	2402	rBV2	38861	46887	1.96%	0.337%
23	18.004	2532	2536	2545	rBV4	45170	85975	3.59%	0.619%
24	18.151	2557	2561	2574	rVB	104368	168918	7.05%	1.216%
25	18.986	2700	2703	2713	rBV2	80198	113636	4.74%	0.818%
26	19.127	2723	2727	2733	rBV	70687	90168	3.76%	0.649%
27	19.504	2784	2791	2797	rBV2	322422	466253	19.46%	3.355%
28	19.680	2816	2821	2826	rBV	1416897	1617623	67.53%	11.641%
29	20.916	3027	3031	3039	rBV3	148254	235385	9.83%	1.694%
30	20.986	3040	3043	3049	rVB	92262	116946	4.88%	0.842%
31	21.116	3062	3065	3070	rVB	103340	111331	4.65%	0.801%
32	21.204	3075	3080	3084	rBV	456041	578495	24.15%	4.163%
33	23.480	3462	3467	3476	rVB2	289344	538158	22.47%	3.873%

Sum of corrected areas: 13896183

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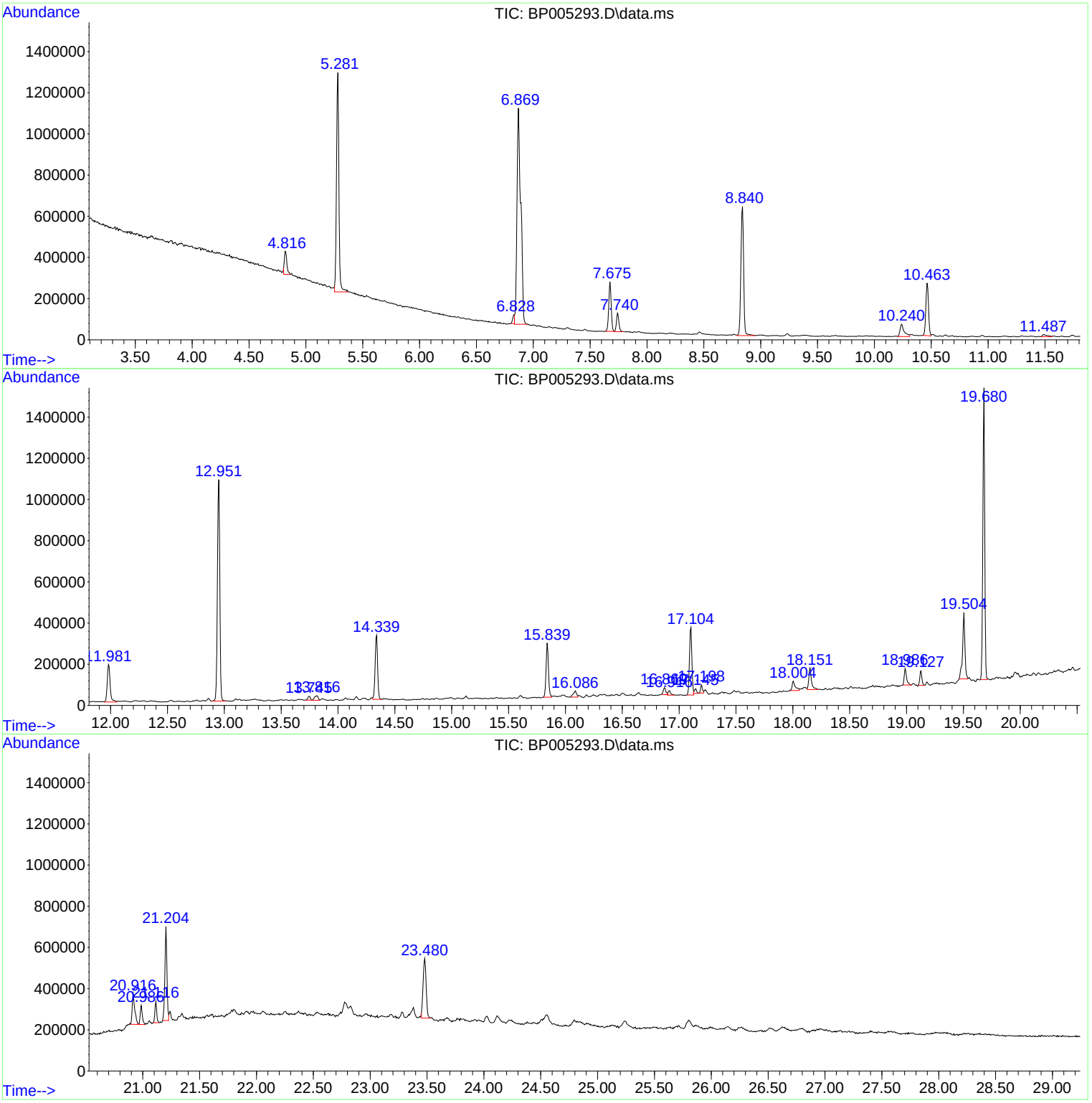
Instrument :
BNA_P
ClientSampleId :
SB-4B

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP040921.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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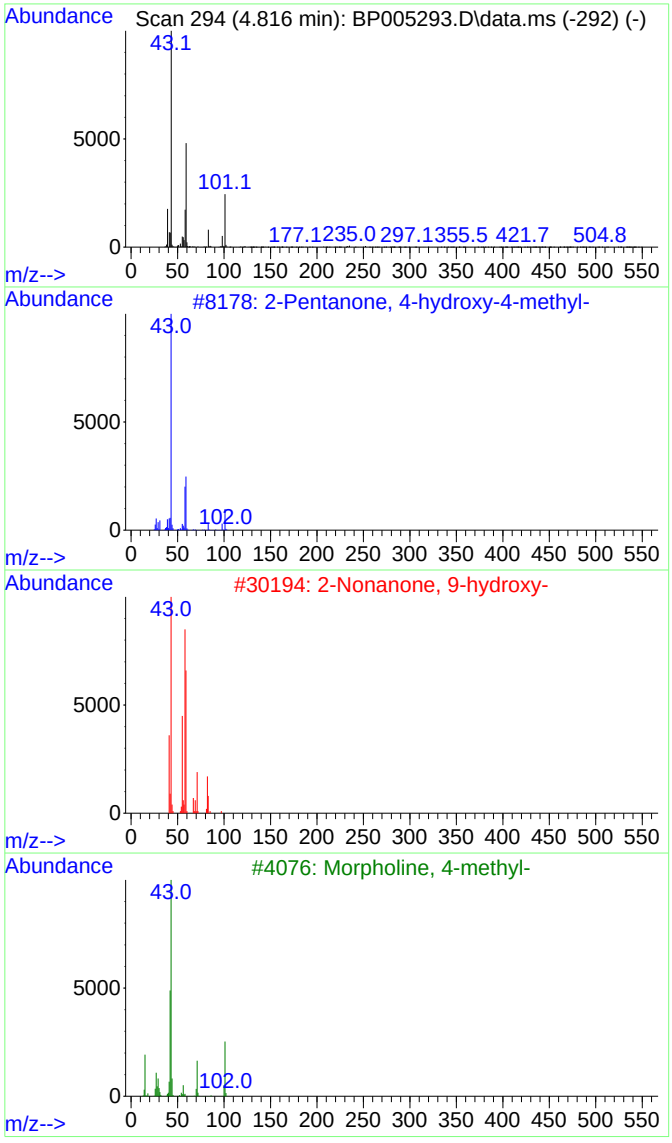
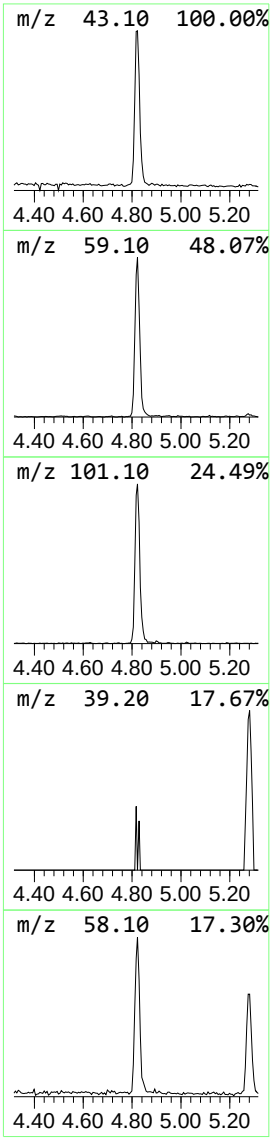
****
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.816	9.22 ng	165249	1,4-Dichlorobenzene-d4	7.675

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	2-Nonanone, 9-hydroxy-	158	C9H18O2	025368-56-3	28
3	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
4	Thiocyanic acid, propyl ester	101	C4H7NS	004251-16-5	9
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9





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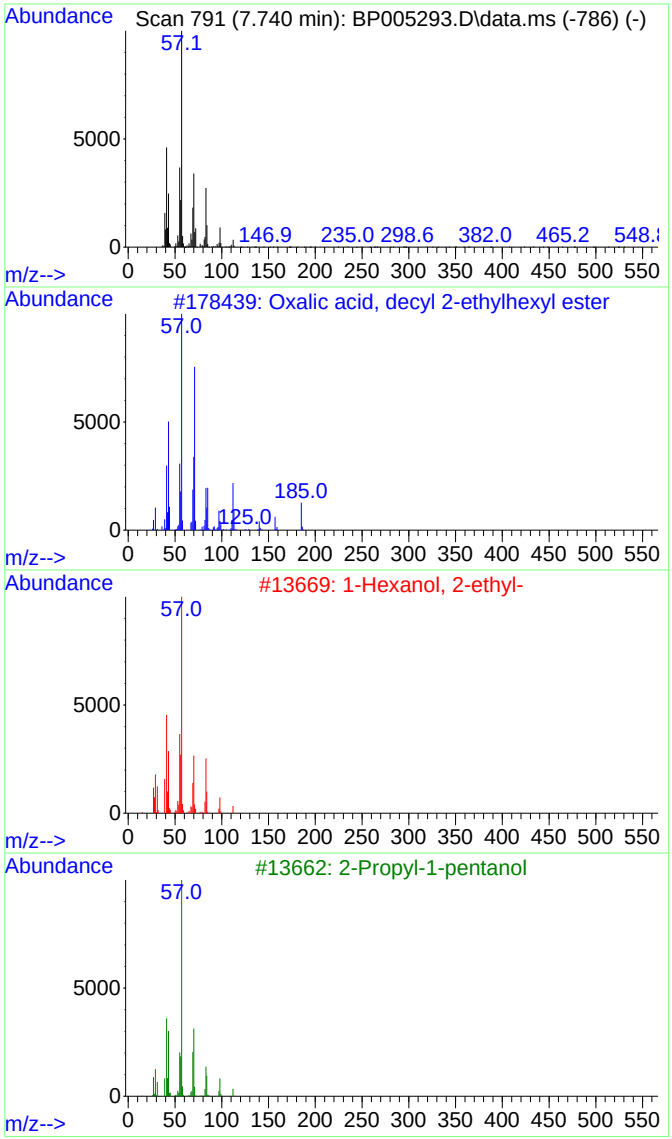
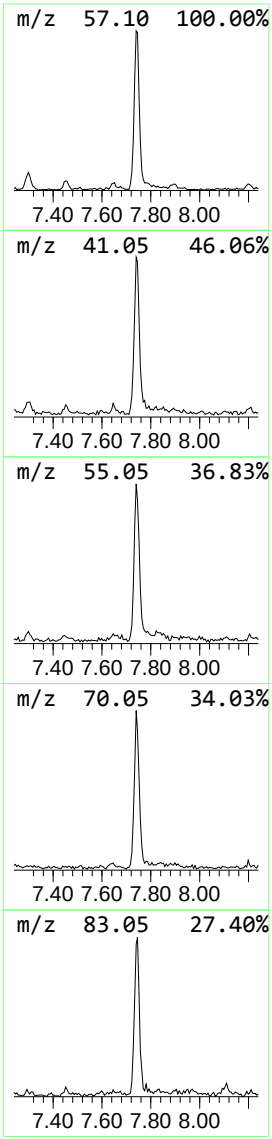
****
Peak Number 2 Oxalic acid, decyl 2-ethylh... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.740	7.59 ng	136138	1,4-Dichlorobenzene-d4	7.675

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oxalic acid, decyl 2-ethylhexyl ...	342	C20H38O4	1000309-39-3	83
2	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	83
3	2-Propyl-1-pentanol	130	C8H18O	058175-57-8	72
4	3-Trifluoroacetoxy-6-ethyldecane	282	C14H25F3O2	116436-59-0	72
5	2-Ethyl-1-hexanol, heptafluorobu...	326	C12H17F7O2	1000365-16-0	59





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Instrument : BNA_P
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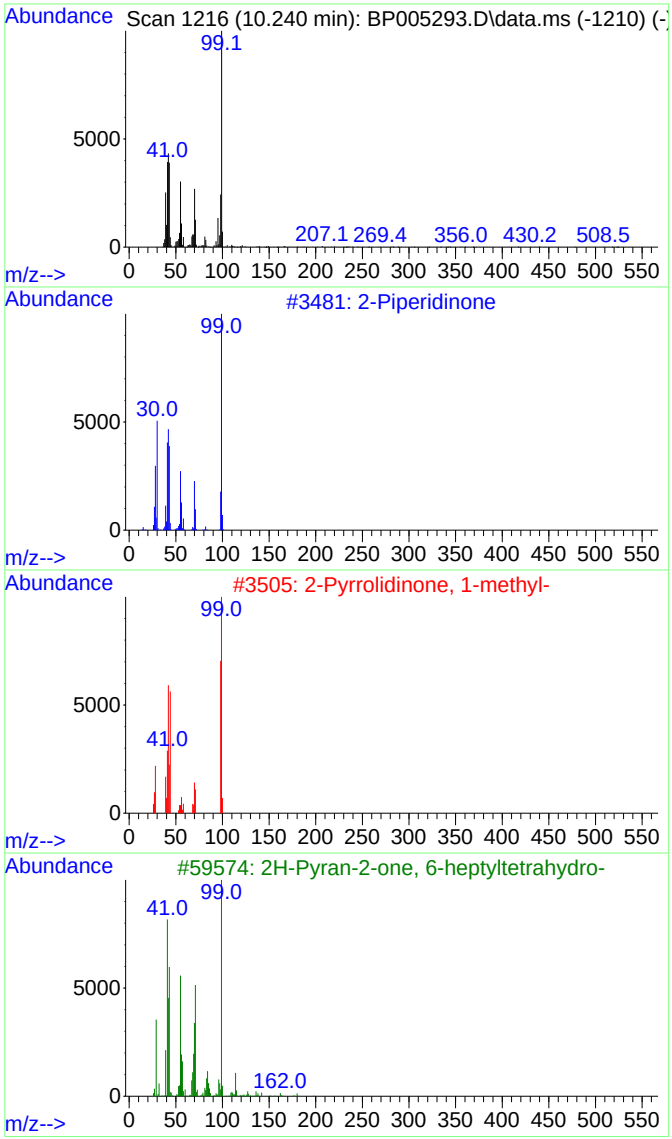
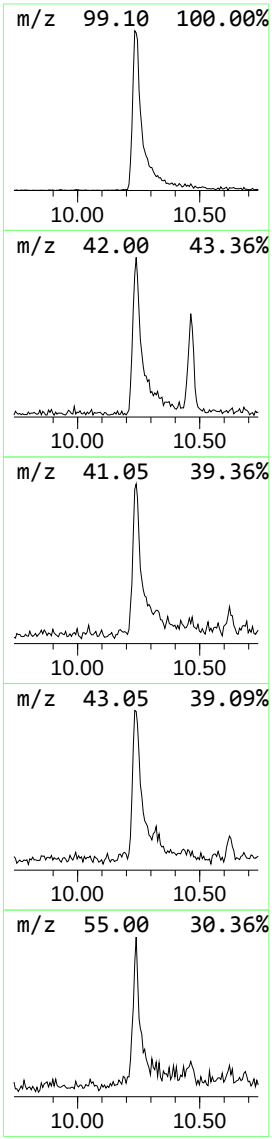
****

Peak Number 3 2-Piperidinone Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.240	7.29 ng	150745	Naphthalene-d8	10.463

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Piperidinone	99	C5H9NO	000675-20-7	87
2	2-Pyrrolidinone, 1-methyl-	99	C5H9NO	000872-50-4	64
3	2H-Pyran-2-one, 6-heptyltetrahydro-	198	C12H22O2	000713-95-1	50
4	2H-Pyran-2-one, tetrahydro-6-pro...	142	C8H14O2	000698-76-0	45
5	5-Amino-3-methyl-1,2,4-oxadiazole	99	C3H5N3O	003663-39-6	40





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Instrument : BNA_P
ClientSampleId : SB-4B

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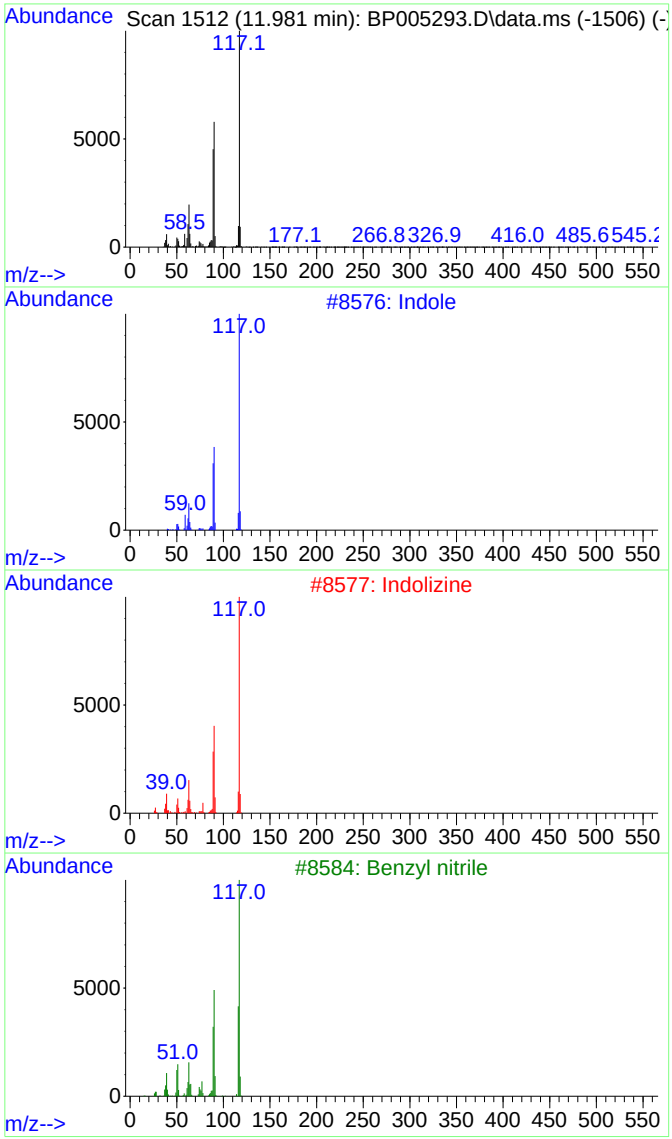
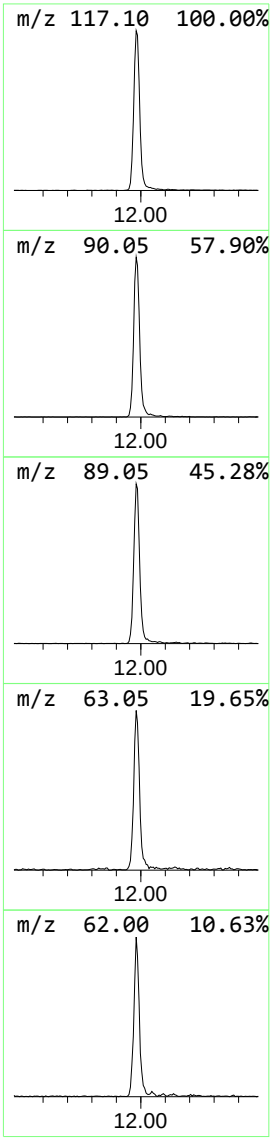
****

Peak Number 4 Indole Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.981	15.39 ng	318350	Naphthalene-d8	10.463

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Indole	117	C8H7N	000120-72-9	95
2	Indolizine	117	C8H7N	000274-40-8	91
3	Benzyl nitrile	117	C8H7N	000140-29-4	91
4	5H-1-Pyrindine	117	C8H7N	000270-91-7	91
5	Benzonitrile, 3-methyl-	117	C8H7N	000620-22-4	91





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Instrument :
BNA_P
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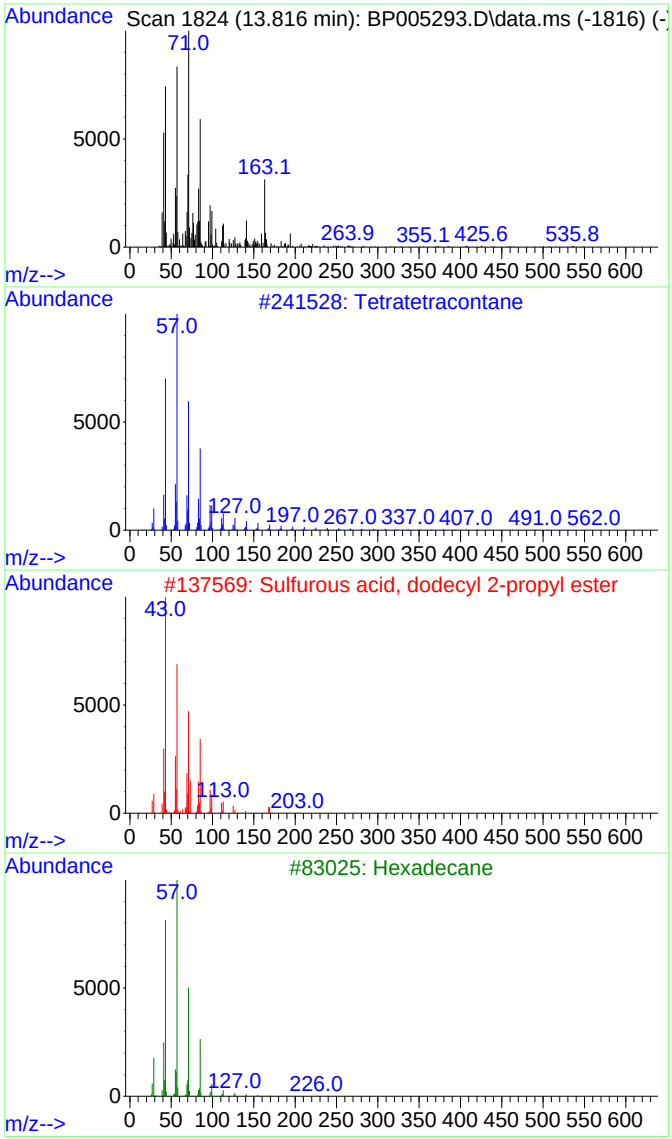
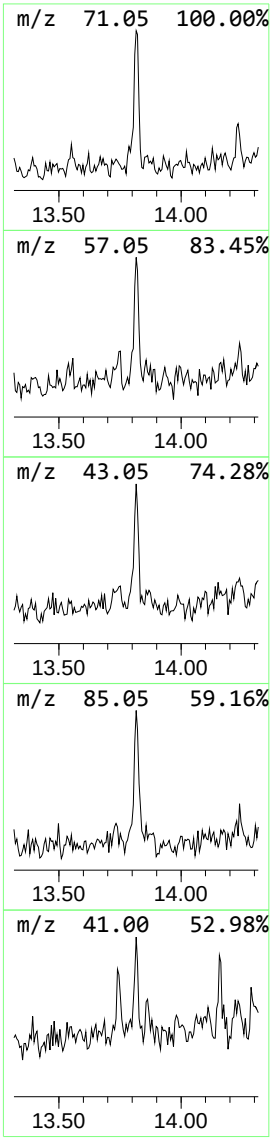
****

Peak Number 5 Tetratetracontane Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.816	2.12 ng	49226	Acenaphthene-d10	14.339

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetratetracontane	619	C44H90	007098-22-8	64
2	Sulfurous acid, dodecyl 2-propyl...	292	C15H32O3S	1000309-12-3	64
3	Hexadecane	226	C16H34	000544-76-3	62
4	Nonadecane, 9-methyl-	282	C20H42	013287-24-6	62
5	Heptadecane, 2,6-dimethyl-	268	C19H40	054105-67-8	53





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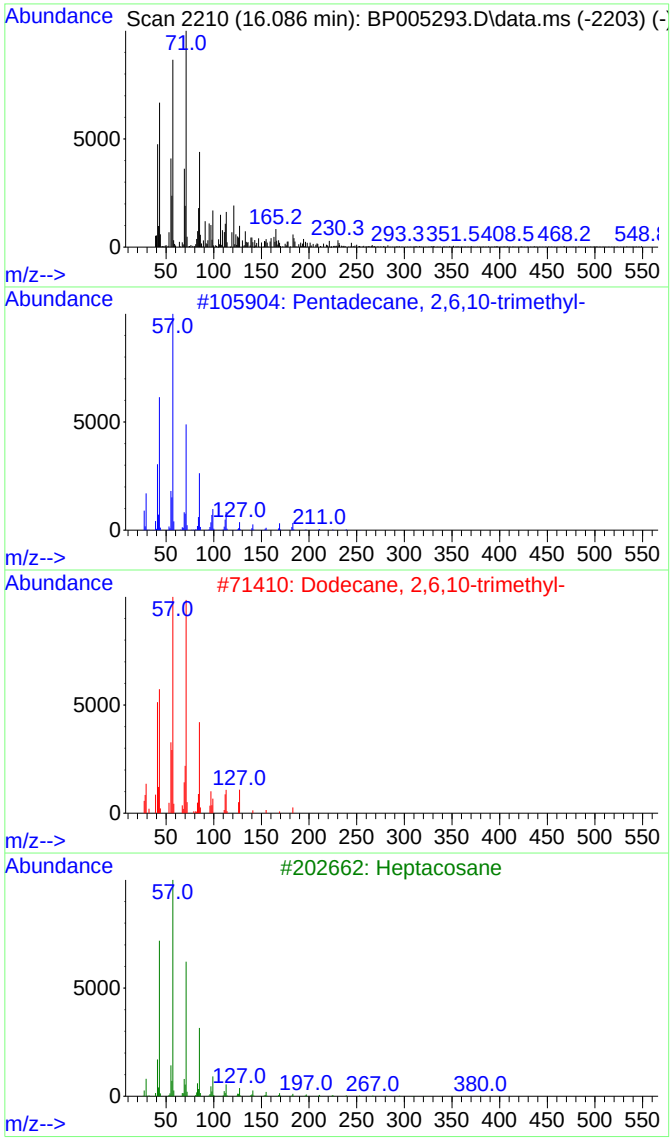
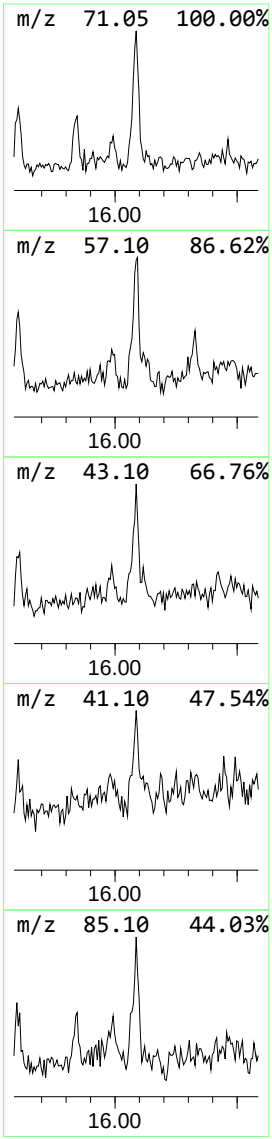
****
Peak Number 6 Pentadecane, 2,6,10-trimethyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.086	2.54 ng	59898	Phenanthrene-d10	17.104

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecane, 2,6,10-trimethyl-	254	C18H38	003892-00-0	87
2	Dodecane, 2,6,10-trimethyl-	212	C15H32	003891-98-3	83
3	Heptacosane	380	C27H56	000593-49-7	83
4	Tetradecane, 4,11-dimethyl-	226	C16H34	055045-12-0	80
5	Heptadecane, 4-methyl-	254	C18H38	026429-11-8	80





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Sample : M1998-06
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_P
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP040921.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
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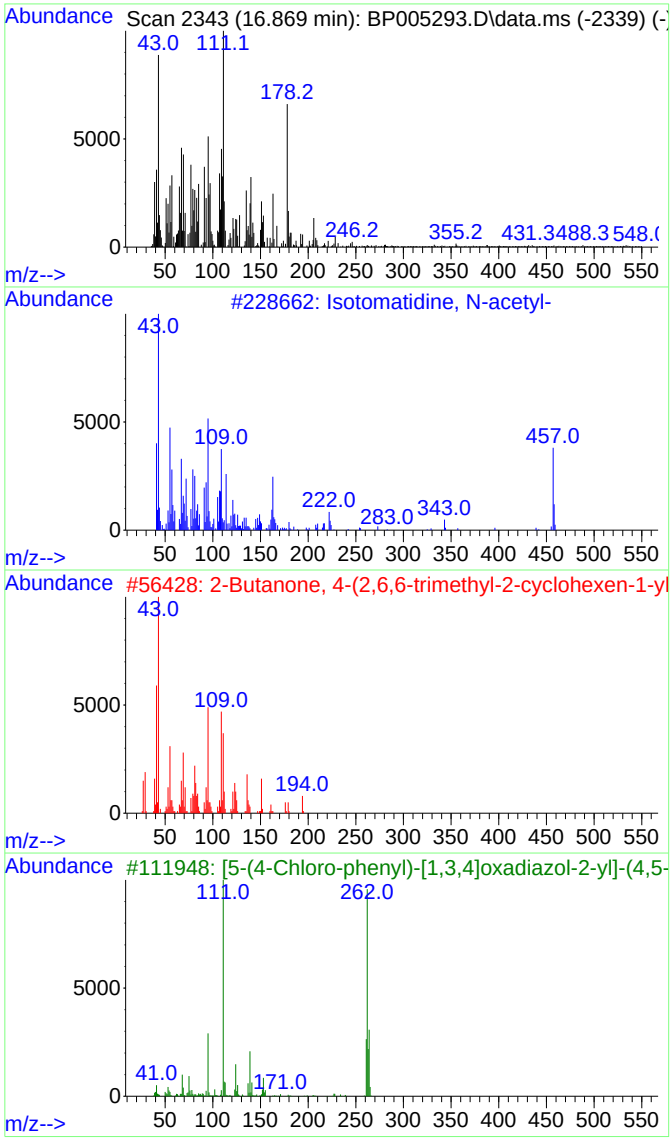
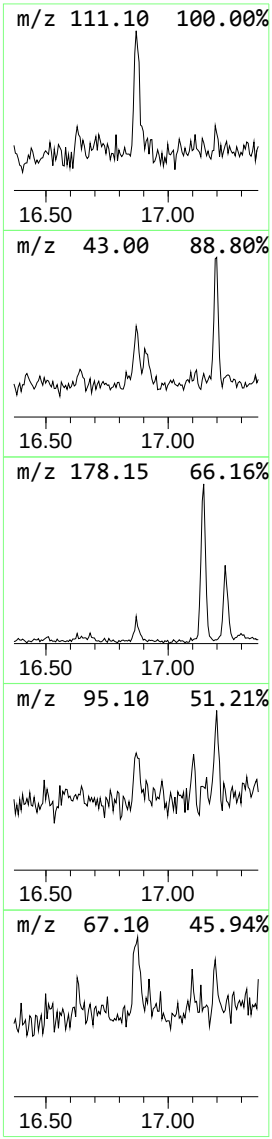
****

Peak Number 7 unknown16.869 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.869	2.33 ng	54950	Phenanthrene-d10	17.104

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Isotomatidine, N-acetyl-	457	C29H47NO3	108990-87-0	35
2	2-Butanone, 4-(2,6,6-trimethyl-2...	194	C13H22O	039721-65-8	30
3	[5-(4-Chloro-phenyl)-[1,3,4]oxad...	262	C12H11ClN4O	1000276-00-3	25
4	Cyclododeca-4,8-dien-1-one, (E,E)-	178	C12H18O	1000163-28-2	18
5	2-Thiophenecarboxylic acid, 2-me...	184	C9H12O2S	116529-98-7	15





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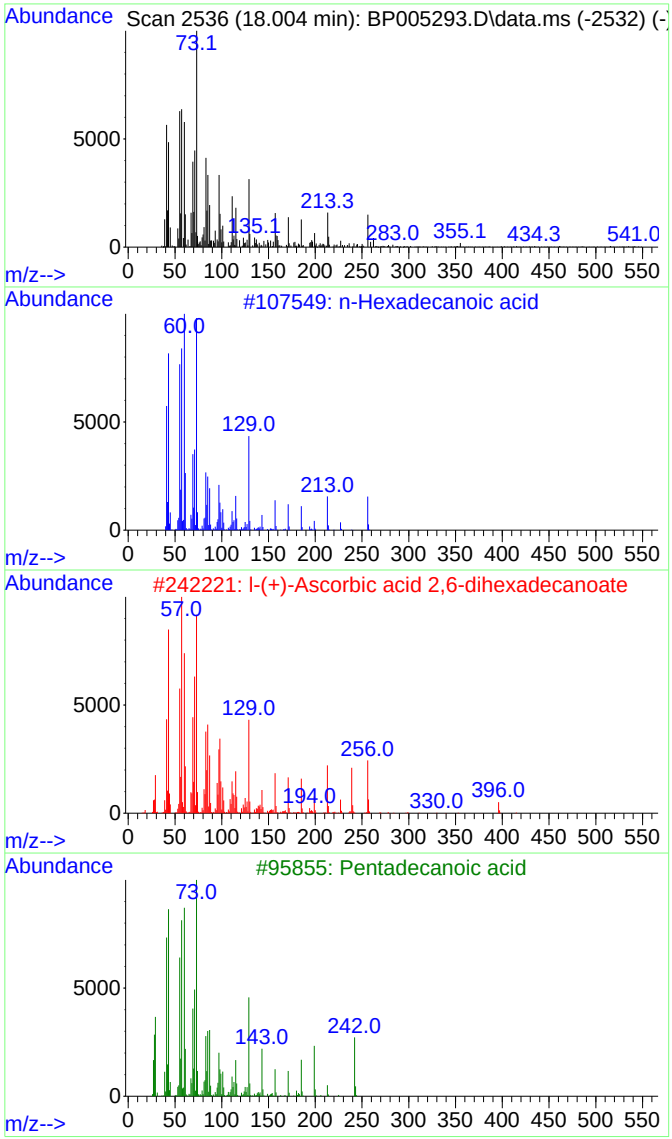
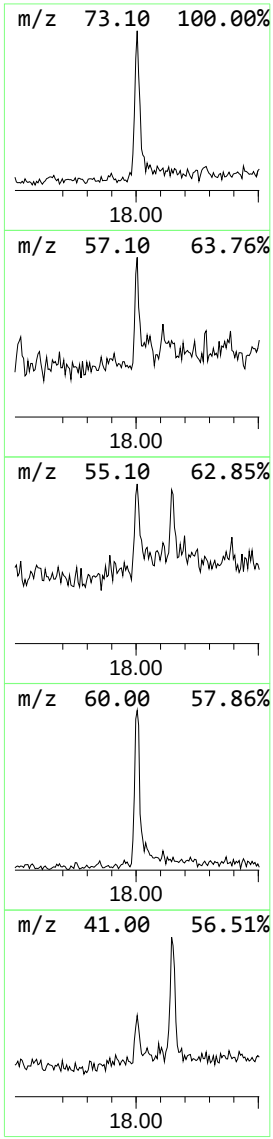
****

Peak Number 8 n-Hexadecanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.004	3.65 ng	85975	Phenanthrene-d10	17.104

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	90
2	l-(+)-Ascorbic acid 2,6-dihexade...	652	C38H68O8	028474-90-0	58
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	52
4	Hexatriacontyl pentafluoropropio...	669	C39H73F5O2	1000351-89-0	49
5	Tetratriacontyl pentafluoropropi...	641	C37H69F5O2	1000351-81-5	46





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TIC Library : C:\DATABASE\NIST11.L
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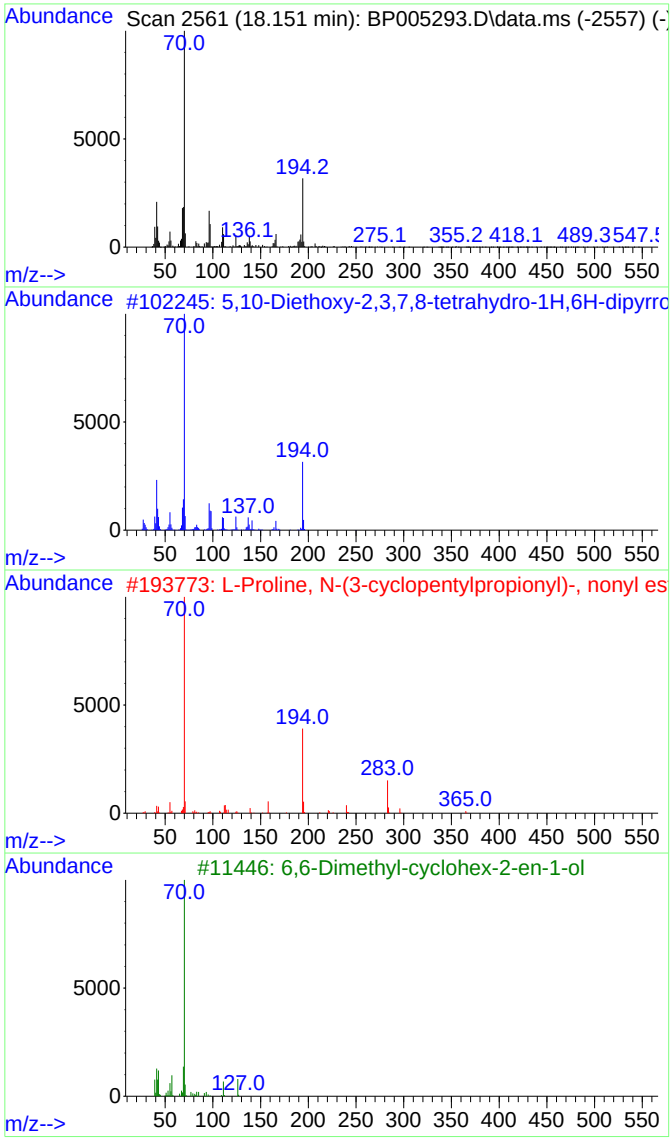
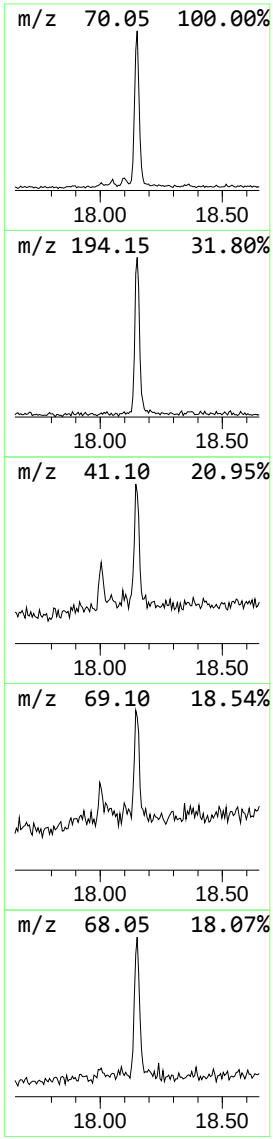
****
Peak Number 9 5,10-Diethoxy-2,3,7,8-tetra... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.151	7.18 ng	168918	Phenanthrene-d10	17.104

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5,10-Diethoxy-2,3,7,8-tetrahydro...	250	C14H22N2O2	1000190-75-5	72
2	L-Proline, N-(3-cyclopentylpropi...	365	C22H39NO3	1000346-41-4	40
3	6,6-Dimethyl-cyclohex-2-en-1-ol	126	C8H14O	038313-10-9	38
4	L-Proline, N-(3-cyclopentylpropi...	323	C19H33NO3	1000346-41-2	33
5	L-Proline, N-(3-cyclopentylpropi...	337	C20H35NO3	1000346-41-3	33





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Data File : BP005293.D
Acq On : 13 Apr 2021 18:34
Operator : CG/JU
Sample : M1998-06
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : SB-4B

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP040921.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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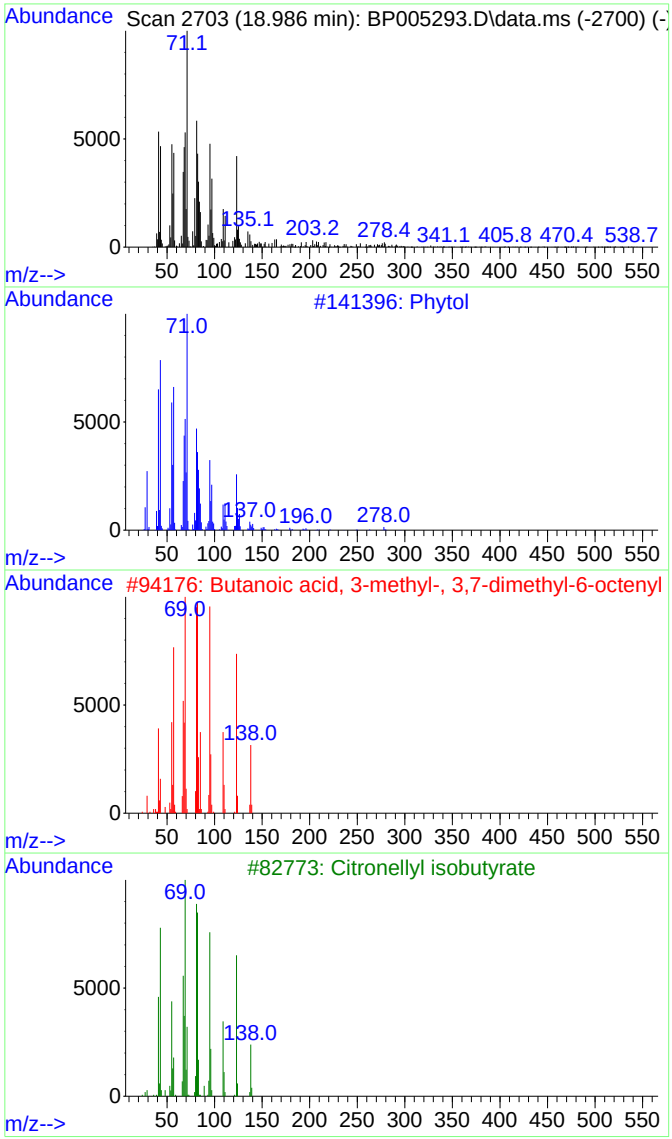
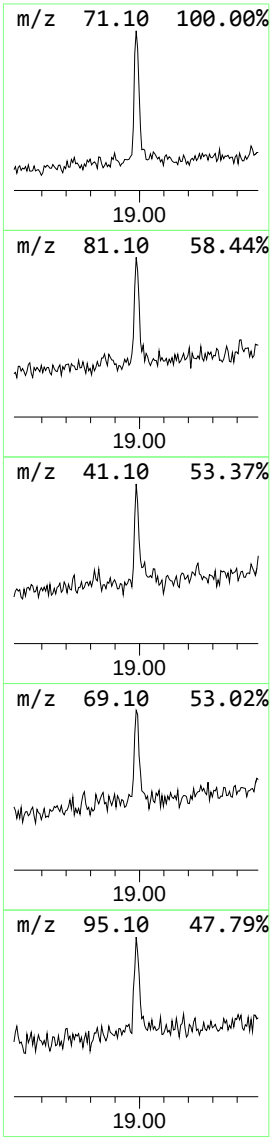
Peak Number 10 Phytol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.986	4.83 ng	113636	Phenanthrene-d10	17.104

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phytol	296	C20H40O	000150-86-7	91
2	Butanoic acid, 3-methyl-, 3,7-di...	240	C15H28O2	068922-10-1	38
3	Citronellyl isobutyrate	226	C14H26O2	000097-89-2	38
4	4-Fluorobenzoic acid, 2-tetrahyd...	224	C12H13FO3	1000279-07-0	38
5	1-Ethynylcyclopentanol	110	C7H10O	017356-19-3	30





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Data File : BP005293.D
Acq On : 13 Apr 2021 18:34
Operator : CG/JU
Sample : M1998-06
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : SB-4B

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP040921.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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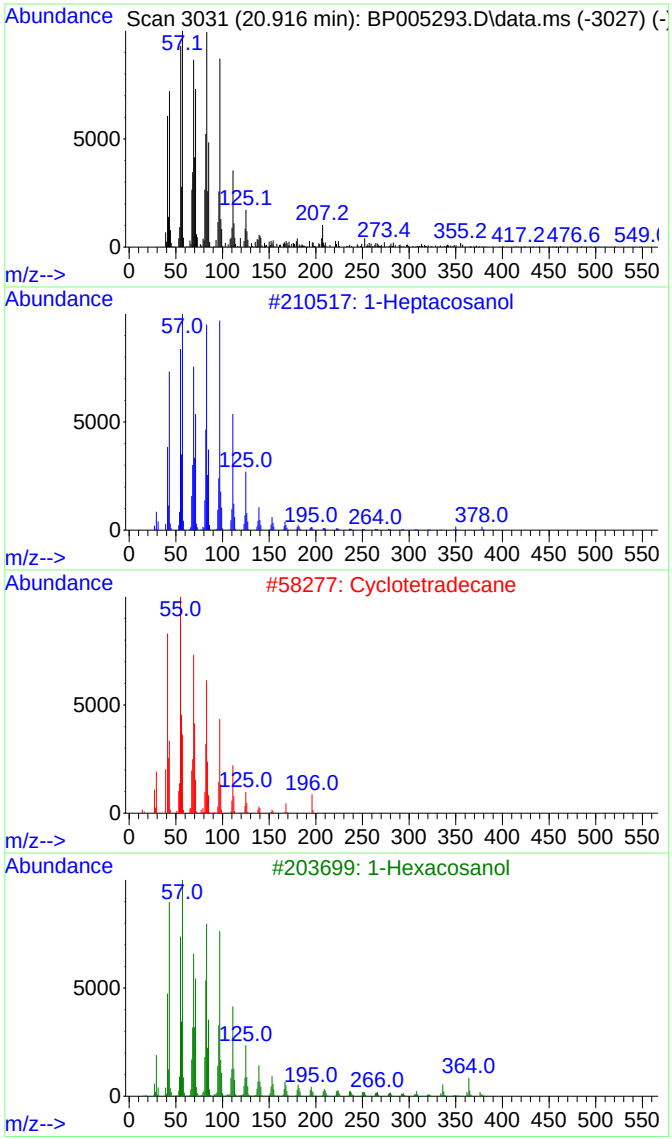
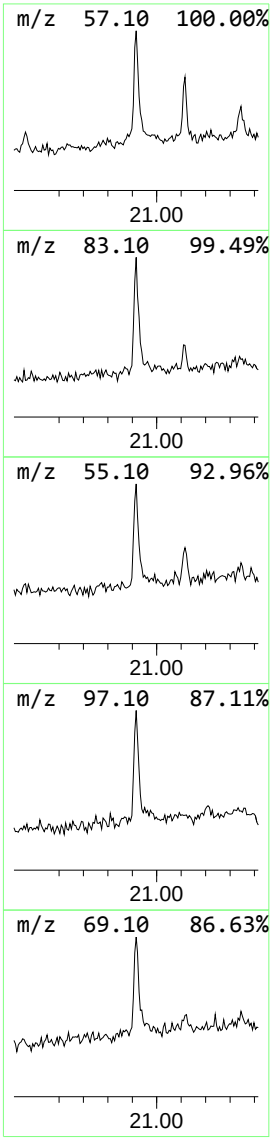
Peak Number 11 1-Heptacosanol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.916	8.14 ng	235385	Chrysene-d12	21.204

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heptacosanol	396	C27H56O	002004-39-9	87
2	Cyclotetradecane	196	C14H28	000295-17-0	76
3	1-Hexacosanol	382	C26H54O	000506-52-5	70
4	1-Triacontanol	438	C30H62O	000593-50-0	68
5	Octacosanol	410	C28H58O	000557-61-9	68





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP041321\
Data File : BP005293.D
Acq On : 13 Apr 2021 18:34
Operator : CG/JU
Sample : M1998-06
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : SB-4B

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP040921.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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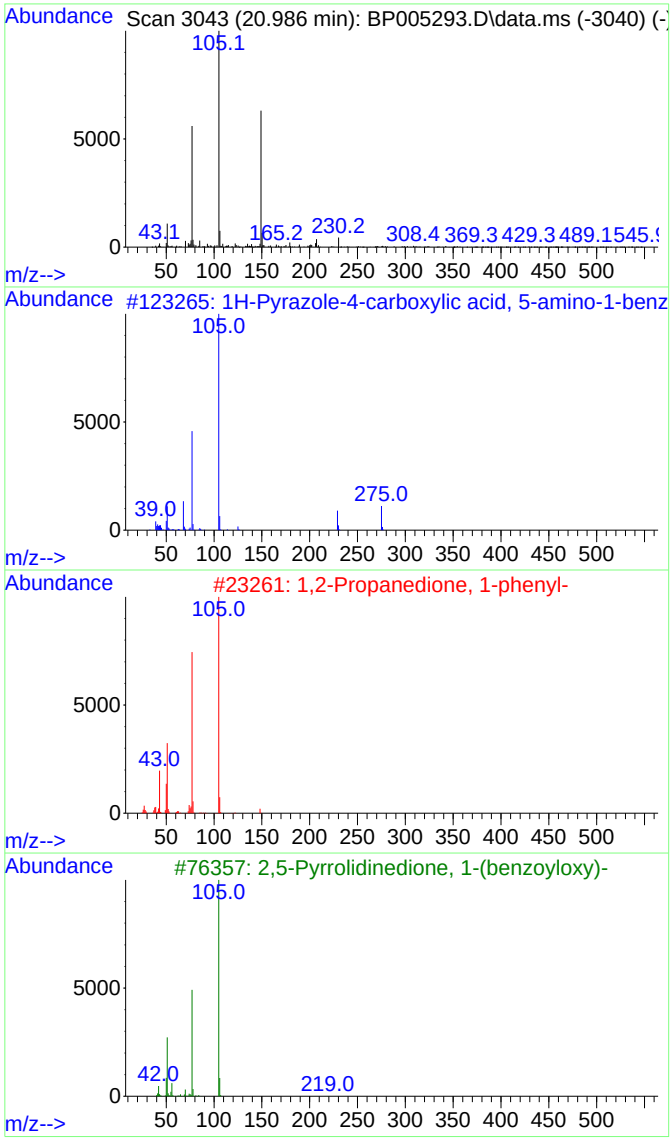
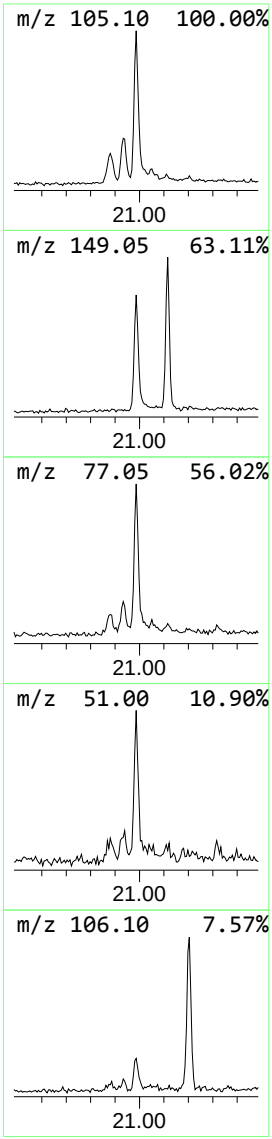
Peak Number 12 unknown20.986 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.986	4.04 ng	116946	Chrysene-d12	21.204

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Pyrazole-4-carboxylic acid, 5...	275	C13H13N3O4	1000315-85-0	47
2	1,2-Propanedione, 1-phenyl-	148	C9H8O2	000579-07-7	43
3	2,5-Pyrrolidinedione, 1-(benzoyl...	219	C11H9NO4	023405-15-4	43
4	N-[1-(3-Benzoyl-4-methyl-5-oxo-o...	350	C20H18N2O4	1000296-93-4	43
5	4'-Nitrobenzanilide	242	C13H10N2O3	003393-96-2	43





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP041321\
Data File : BP005293.D
Acq On : 13 Apr 2021 18:34
Operator : CG/JU
Sample : M1998-06
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : SB-4B

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP040921.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
2-Pentanone, 4-...	4.816	9.2	ng	165249	1	7.675	358571	20.0
Oxalic acid, de...	7.740	7.6	ng	136138	1	7.675	358571	20.0
2-Piperidinone	10.240	7.3	ng	150745	2	10.463	413646	20.0
Indole	11.981	15.4	ng	318350	2	10.463	413646	20.0
Tetratetracontane	13.816	2.1	ng	49226	3	14.339	464572	20.0
Pentadecane, 2,...	16.086	2.5	ng	59898	4	17.104	470786	20.0
unknown16.869	16.869	2.3	ng	54950	4	17.104	470786	20.0
n-Hexadecanoic ...	18.004	3.6	ng	85975	4	17.104	470786	20.0
5,10-Diethoxy-2...	18.151	7.2	ng	168918	4	17.104	470786	20.0
Phytol	18.986	4.8	ng	113636	4	17.104	470786	20.0
1-Heptacosanol	20.916	8.1	ng	235385	5	21.204	578495	20.0
unknown20.986	20.986	4.0	ng	116946	5	21.204	578495	20.0