LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP110920\
Data File : BP003875.D
Acq On : 09 Nov 2020 19:05
Operator : CG/JU
Sample : L4658-06
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
1998-OS

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\8270-BP110320.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP003875.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.946	5	10	29	rVB	5759886	6392075	100.00%	15.315%
2	3.105	30	37	47	rVV	114477	220728	3.45%	0.529%
3	3.193	47	52	61	rVB	333841	381834	5.97%	0.915%
4	5.816	491	498	514	rBV	1839440	2771354	43.36%	6.640%
5	7.463	767	778	795	rBV	1735664	2797494	43.77%	6.703%
6	8.299	910	920	928	rBV	586703	934806	14.62%	2.240%
7	9.463	1110	1118	1127	rBV	1117976	1804550	28.23%	4.324%
8	11.134	1394	1402	1412	rBV	687877	1192812	18.66%	2.858%
9	13.540	1805	1811	1821	rBV	2448831	3690884	57.74%	8.843%
10	13.734	1840	1844	1851	rBV2	106943	179095	2.80%	0.429%
11	14.257	1930	1933	1936	rBV4	58547	65409	1.02%	0.157%
12	14.363	1943	1951	1955	rBV2	477062	858179	13.43%	2.056%
13	14.475	1967	1970	1978	rVB	116819	212208	3.32%	0.508%
14	14.681	2000	2005	2011	rBV4	294657	690801	10.81%	1.655%
15	14.728	2011	2013	2015	rVV3	128987	149062	2.33%	0.357%
16	14.763	2015	2019	2025	rVB	696496	1066848	16.69%	2.556%
17	14.840	2029	2032	2037	rVB3	122968	152636	2.39%	0.366%
18	14.916	2037	2045	2056	rVB3	1073162	2091326	32.72%	5.011%
19	15.022	2059	2063	2067	rBV3	195211	347108	5.43%	0.832%
20	15.428	2128	2132	2137	rBV3	175470	342926	5.36%	0.822%
21	15.587	2156	2159	2163	rVB	291118	346220	5.42%	0.830%
22	15.716	2177	2181	2186	rVB	795276	1093488	17.11%	2.620%
23	16.398	2292	2297	2301	rBV	1639752	2416099	37.80%	5.789%
24	16.628	2332	2336	2342	rVB2	895411	1286607	20.13%	3.083%
25	17.645	2506	2509	2518	rVB	1039723	1634498	25.57%	3.916%
26	20.139	2929	2933	2941	rVB	3559559	4438929	69.44%	10.635%
27	21.322	3132	3134	3145	rVB	517449	794567	12.43%	1.904%
28	21.669	3190	3193	3199	rVB	1162117	1528920	23.92%	3.663%
29	23.298	3466	3470	3474	rVB	146562	210295	3.29%	0.504%
30	24.151	3608	3615	3624	rVB	789249	1645911	25.75%	3.943%

Sum of corrected areas: 41737669

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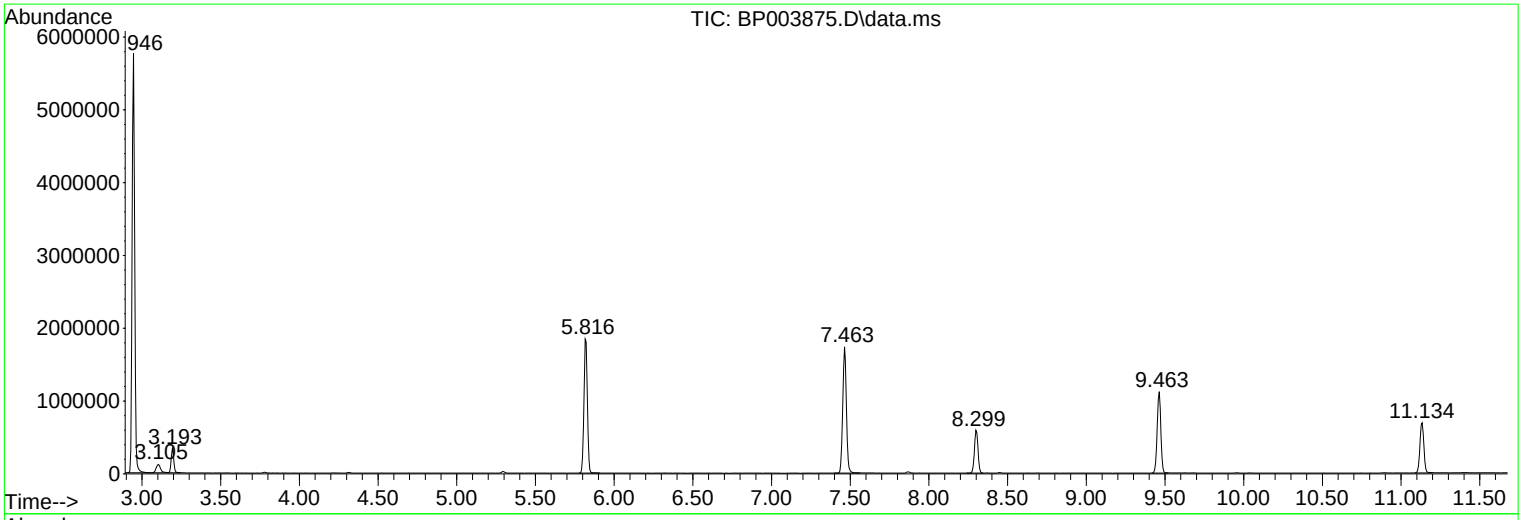
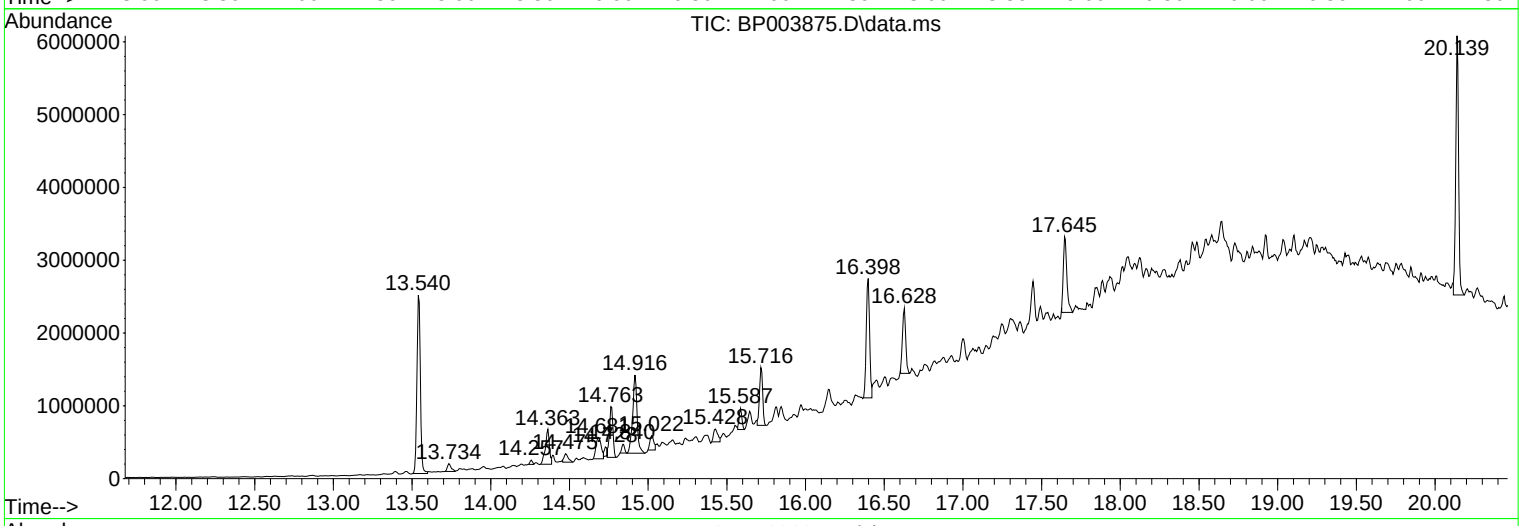
Sample : L4658-06
Misc :
ALS Vial : 17 Sample Multiplier: 1

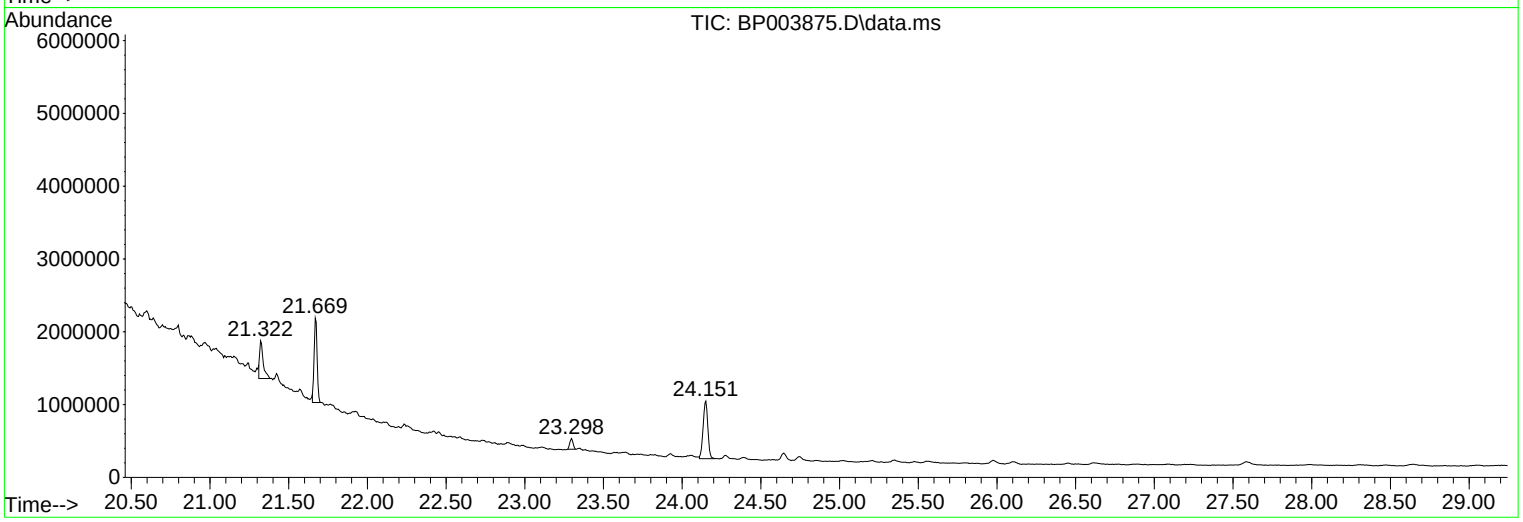
Instrument :
BNA_P
ClientSampleId :
1998-OS

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP110320.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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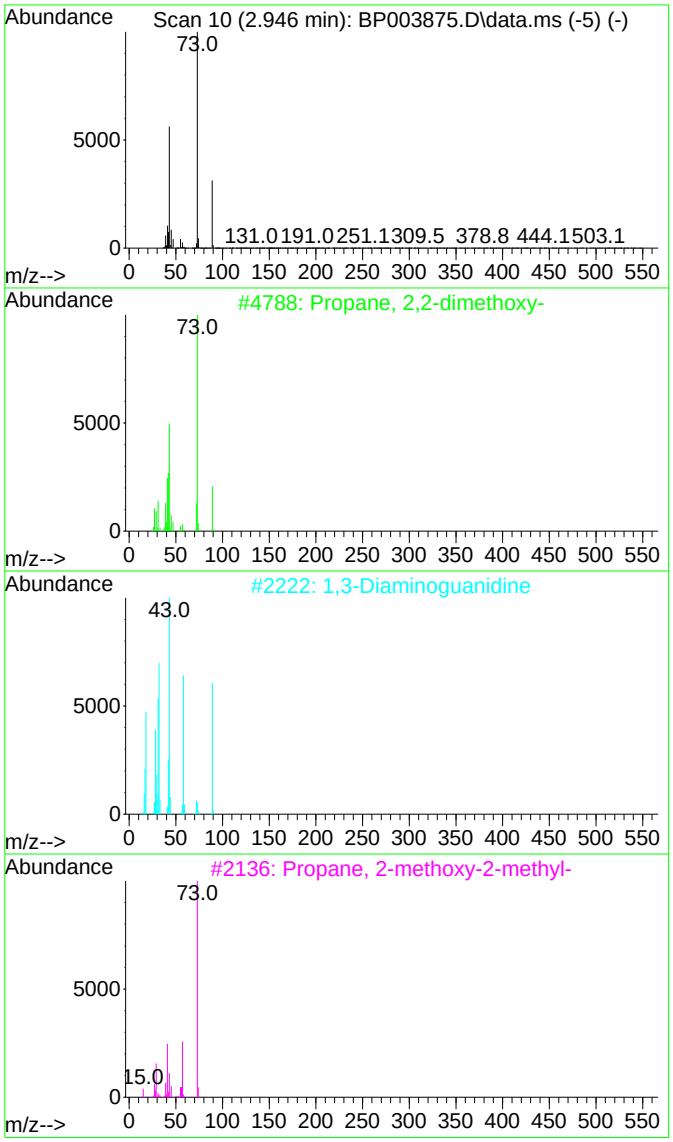
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

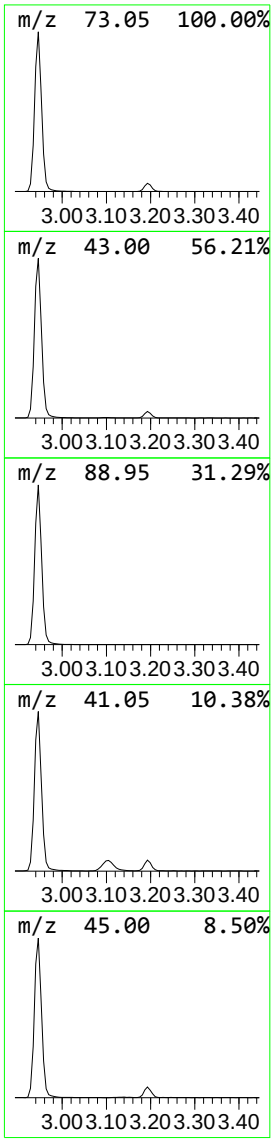
****

Peak Number 1 unknown2.946 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.946	136.76 ng	6392080	1,4-Dichlorobenzene-d4	8.299

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 2,2-dimethoxy-	104	C5H12O2	000077-76-9	38
2	1,3-Diaminoguanidine	89	CH7N5	004364-78-7	9
3	Propane, 2-methoxy-2-methyl-	88	C5H12O	001634-04-4	9
4	1-Hexen-4-ol, 1-chloro-3,5-dimet...	162	C8H15ClO	100244-09-5	9
5	2-Hydroxy-2-methylbutyric acid	118	C5H10O3	003739-30-8	9





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Operator : CG/JU
Sample : L4658-06
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
1998-OS

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP110320.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
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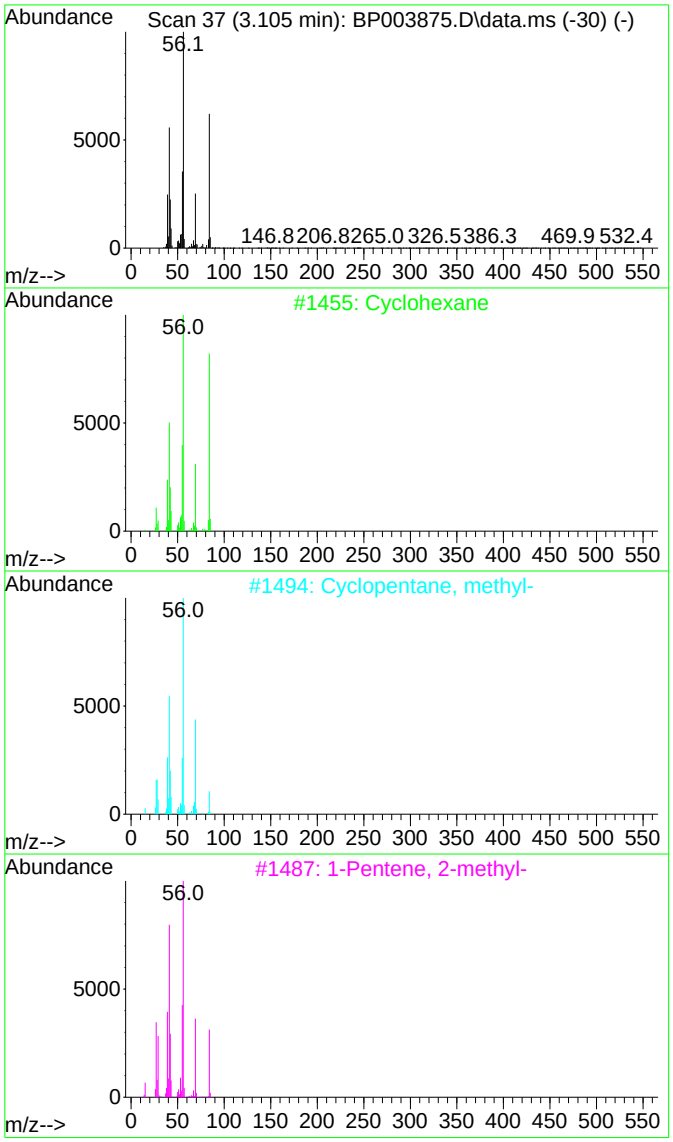
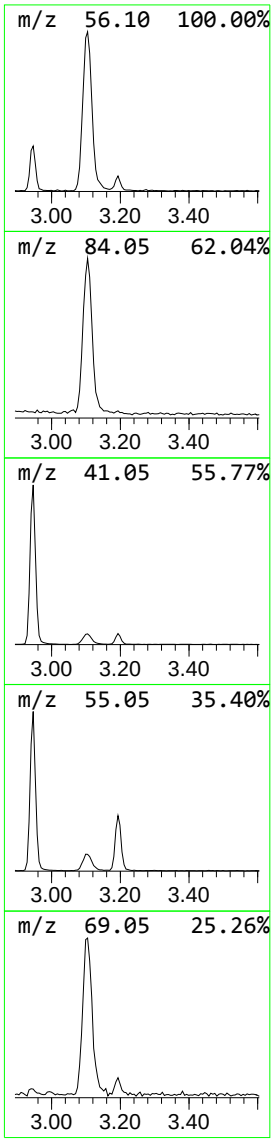
Peak Number 2 Cyclohexane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.105	4.72 ng	220728	1,4-Dichlorobenzene-d4	8.299

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexane	84	C6H12	000110-82-7	95
2	Cyclopentane, methyl-	84	C6H12	000096-37-7	50
3	1-Pentene, 2-methyl-	84	C6H12	000763-29-1	49
4	1-Butanol	74	C4H10O	000071-36-3	47
5	2-Acetylpiperidine	127	C7H13NO	097073-22-8	45





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Operator : CG/JU
Sample : L4658-06
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
1998-OS

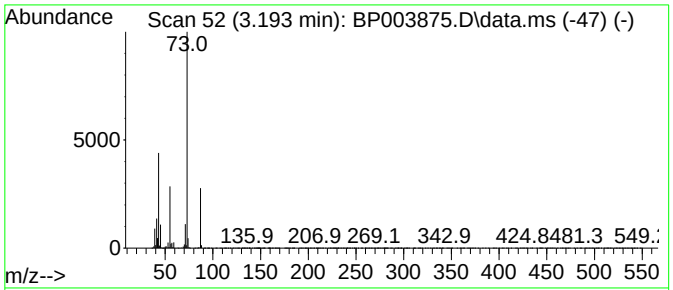
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP110320.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

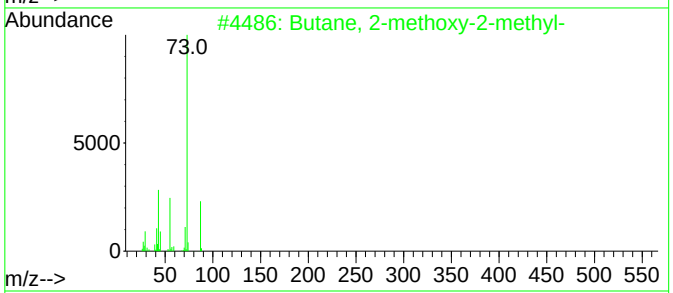
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

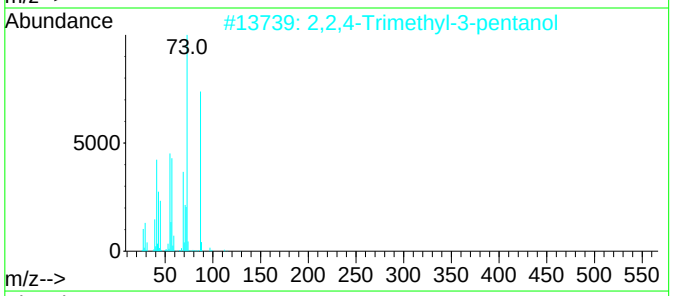
****
Peak Number 3 Butane, 2-methoxy-2-methyl- Concentration Rank 6

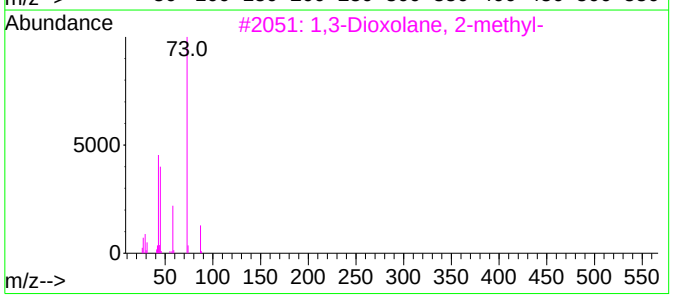
R.T.	EstConc	Area	Relative to ISTD	R.T.
3.193	8.17 ng	381834	1,4-Dichlorobenzene-d4	8.299

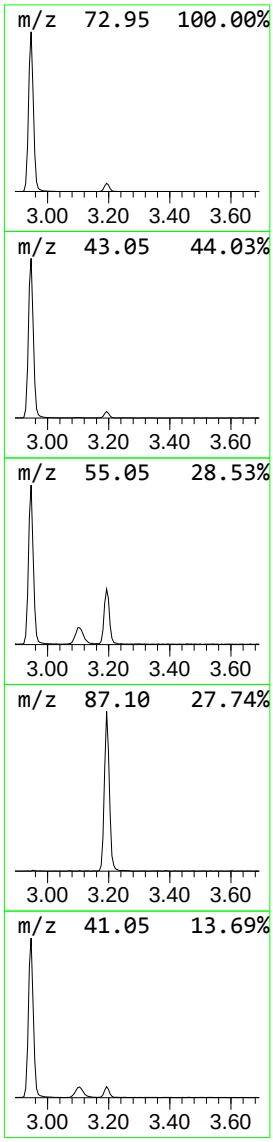
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	23
4	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12
5	N-Ethylformamide	73	C3H7NO	000627-45-2	9











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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP110320.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

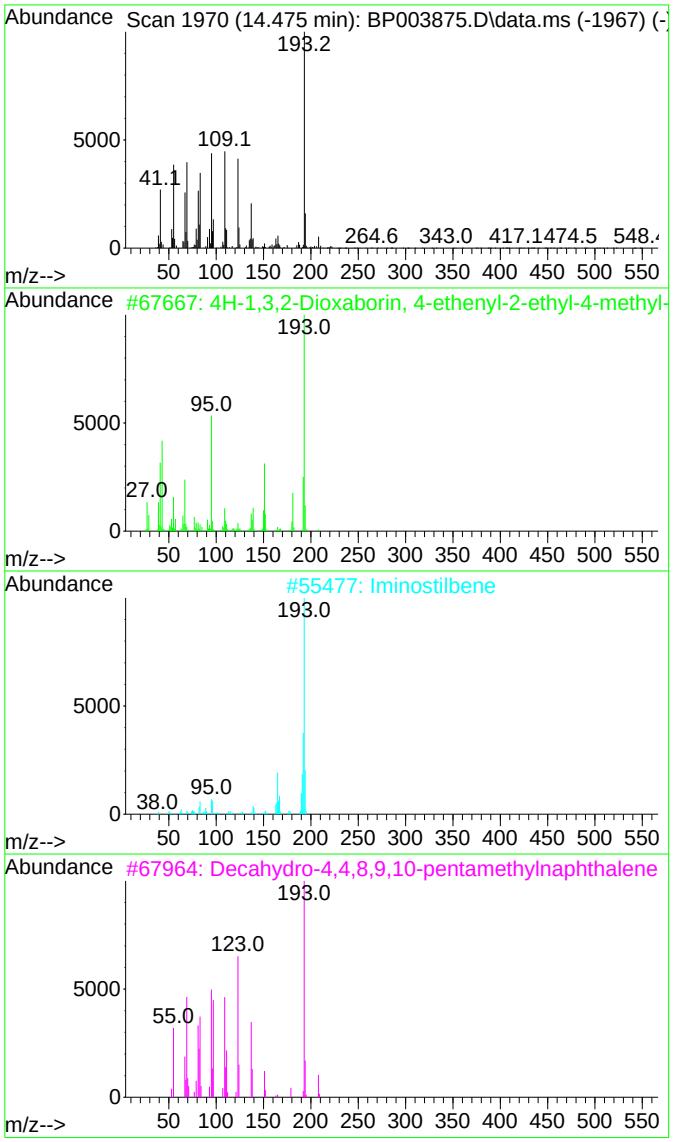
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

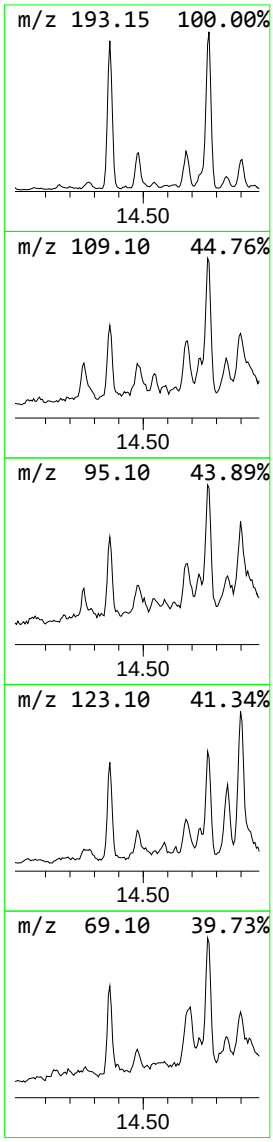
****

Peak Number 4 unknown14.475 Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.475	2.03 ng	212208	Acenaphthene-d10	14.916

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-1,3,2-Dioxaborin, 4-ethenyl-2...	208	C12H21BO2	074630-04-9	37
2	Iminostilbene	193	C14H11N	000256-96-2	30
3	Decahydro-4,4,8,9,10-pentamethyl...	208	C15H28	080655-44-3	30
4	1-Anthracenamine	193	C14H11N	000610-49-1	22
5	Acridine, 9-methyl-	193	C14H11N	000611-64-3	22





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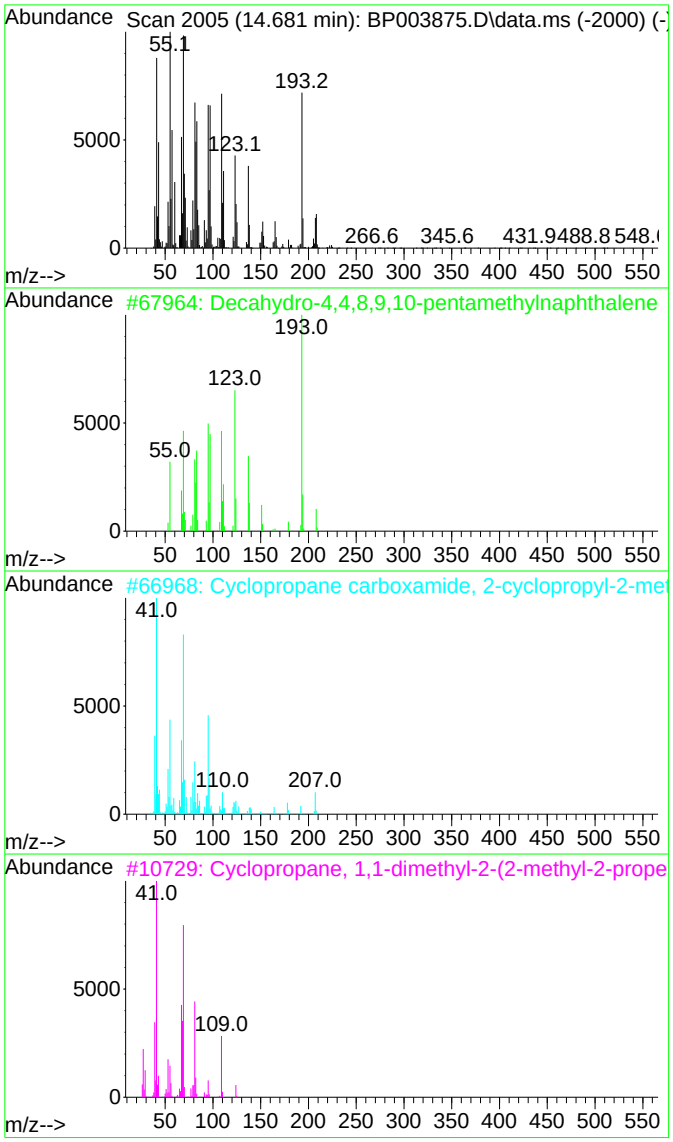
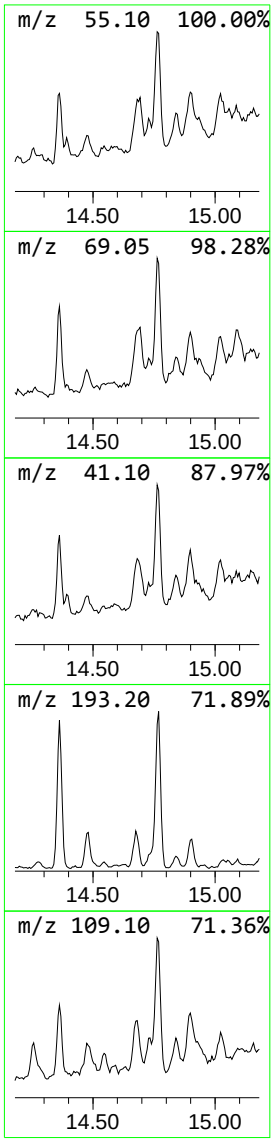
Peak Number 5 unknown14.681 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.681	6.61 ng	690801	Acenaphthene-d10	14.916

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Decahydro-4,4,8,9,10-pentamethyl...	208	C15H28	080655-44-3	46
2	Cyclopropane carboxamide, 2-cycl...	207	C13H21NO	331416-19-4	42
3	Cyclopropane, 1,1-dimethyl-2-(2-...	124	C9H16	069147-03-1	41
4	Borinic acid, diethyl-, 3,3,5-tr...	208	C13H25BO	057387-76-5	25
5	Cyclohexane, 1,2-dimethyl-3-pent...	224	C16H32	062376-17-4	25





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TIC Library : C:\DATABASE\NIST11.L
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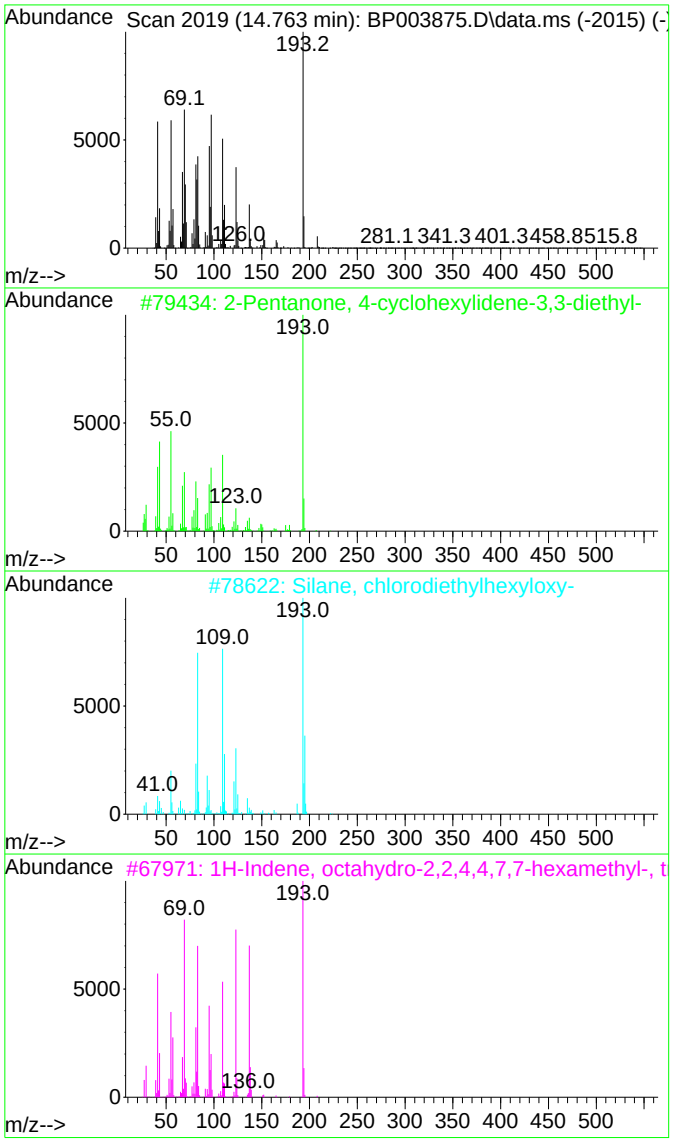
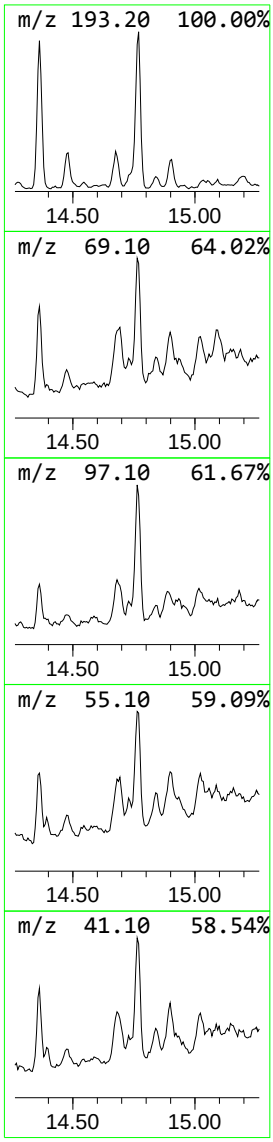
Peak Number 6 unknown14.763 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.763	10.20 ng	1066850	Acenaphthene-d10	14.916

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-cyclohexylidene-3...	222	C15H26O	313253-65-5	40
2	Silane, chlorodiethylhexyloxy-	222	C10H23ClOSi	1000363-74-4	40
3	1H-Indene, octahydro-2,2,4,4,7,7...	208	C15H28	054832-83-6	38
4	Decahydro-4,4,8,9,10-pentamethyl...	208	C15H28	080655-44-3	37
5	Borinic acid, diethyl-, 3,3,5-tr...	208	C13H25BO	057387-76-5	23





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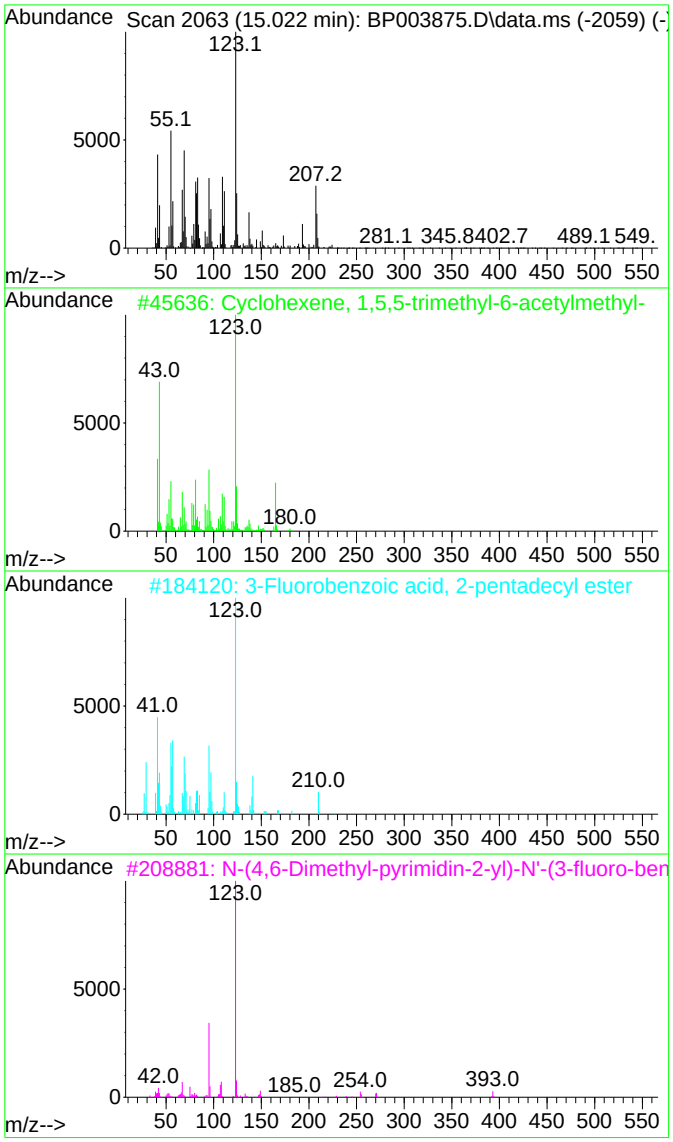
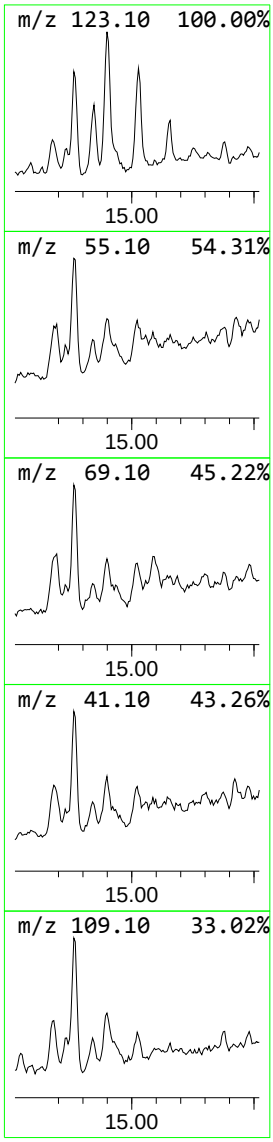
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Cyclohexene, 1,5,5-trimethy... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.022	3.32 ng	347108	Acenaphthene-d10	14.916

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexene, 1,5,5-trimethyl-6-a...	180	C12H20O	211563-96-1	52
2	3-Fluorobenzoic acid, 2-pentadec...	350	C22H35FO2	1000280-60-7	37
3	N-(4,6-Dimethyl-pyrimidin-2-yl)-...	393	C21H20FN5O2	1000300-88-4	35
4	4-Fluorobenzoic acid, 2-methylph...	230	C14H11FO2	1000299-05-3	35
5	3-(2-Ethyl-imidazol-1-yl)-propio...	168	C8H12N2O2	1000277-78-0	32





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TIC Library : C:\DATABASE\NIST11.L
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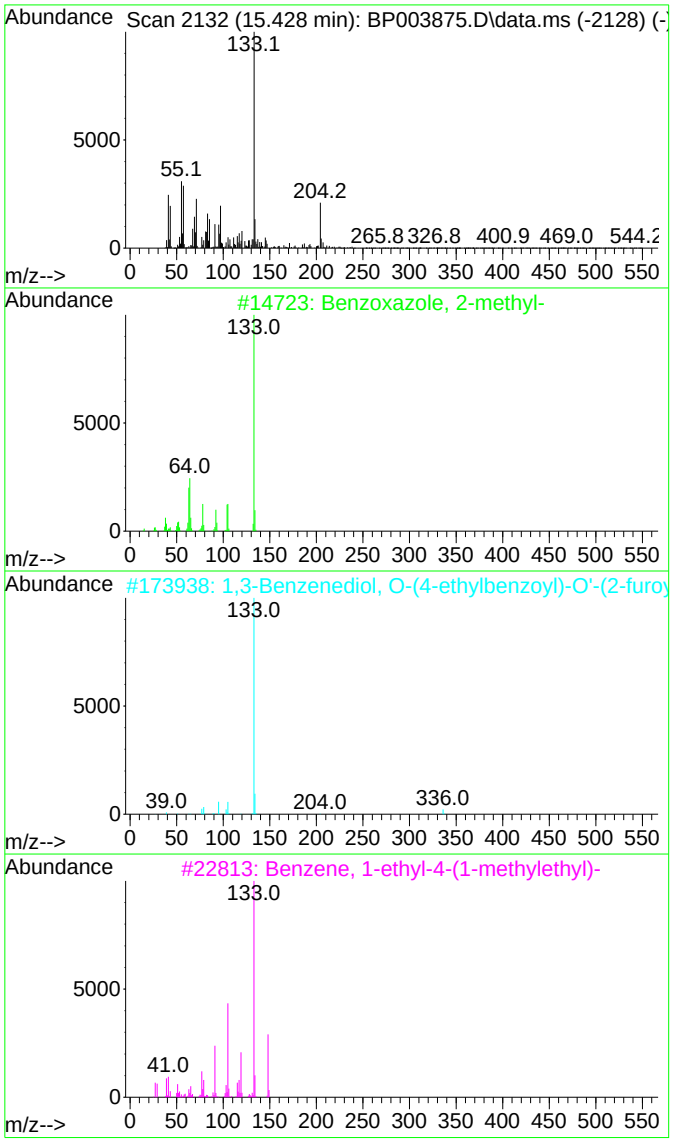
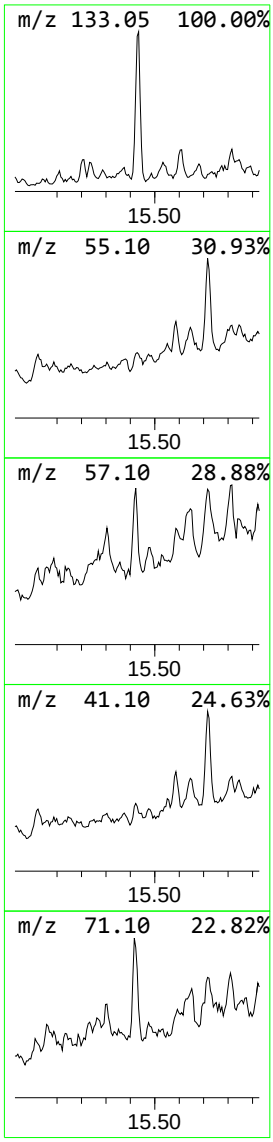
Peak Number 8 unknown15.428 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.428	3.28 ng	342926	Acenaphthene-d10	14.916

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzoxazole, 2-methyl-	133	C8H7NO	000095-21-6	43
2	1,3-Benzenediol, O-(4-ethylbenzo...	336	C20H16O5	1000345-53-5	43
3	Benzene, 1-ethyl-4-(1-methylethyl)-	148	C11H16	004218-48-8	38
4	1-(3-Methylbutyl)-2,4,6-trimethy...	190	C14H22	016204-65-2	38
5	1,2-Benzenediol, o-(2-bromopropi...	376	C18H17BrO4	1000325-97-0	38





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Data File : BP003875.D
Acq On : 09 Nov 2020 19:05
Operator : CG/JU
Sample : L4658-06
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
1998-OS

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP110320.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

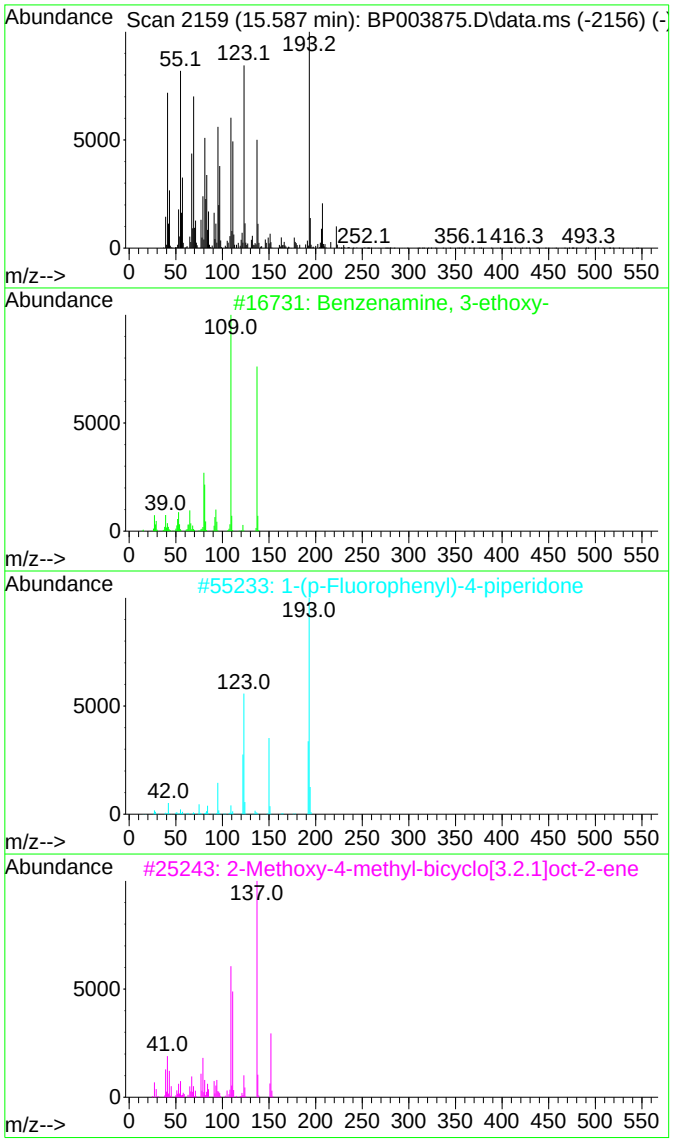
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

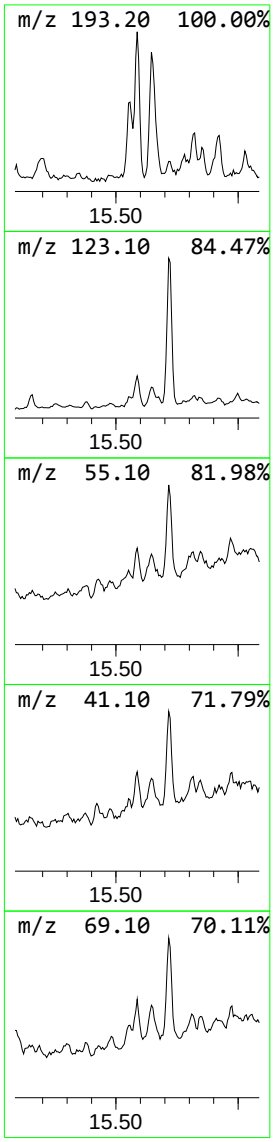
****

Peak Number 9 unknown15.586 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.586	3.31 ng	346220	Acenaphthene-d10	14.916

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzenamine, 3-ethoxy-	137	C8H11NO	000621-33-0	25
2	1-(p-Fluorophenyl)-4-piperidone	193	C11H12FNO	1000238-56-7	25
3	2-Methoxy-4-methyl-bicyclo[3.2.1...	152	C10H16O	1000188-09-4	20
4	6-Methylphenanthridine	193	C14H11N	003955-65-5	11
5	5-Ethoxy-2-methyl-pyridine	137	C8H11NO	055270-48-9	11





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BNA_P
ClientSampleId :
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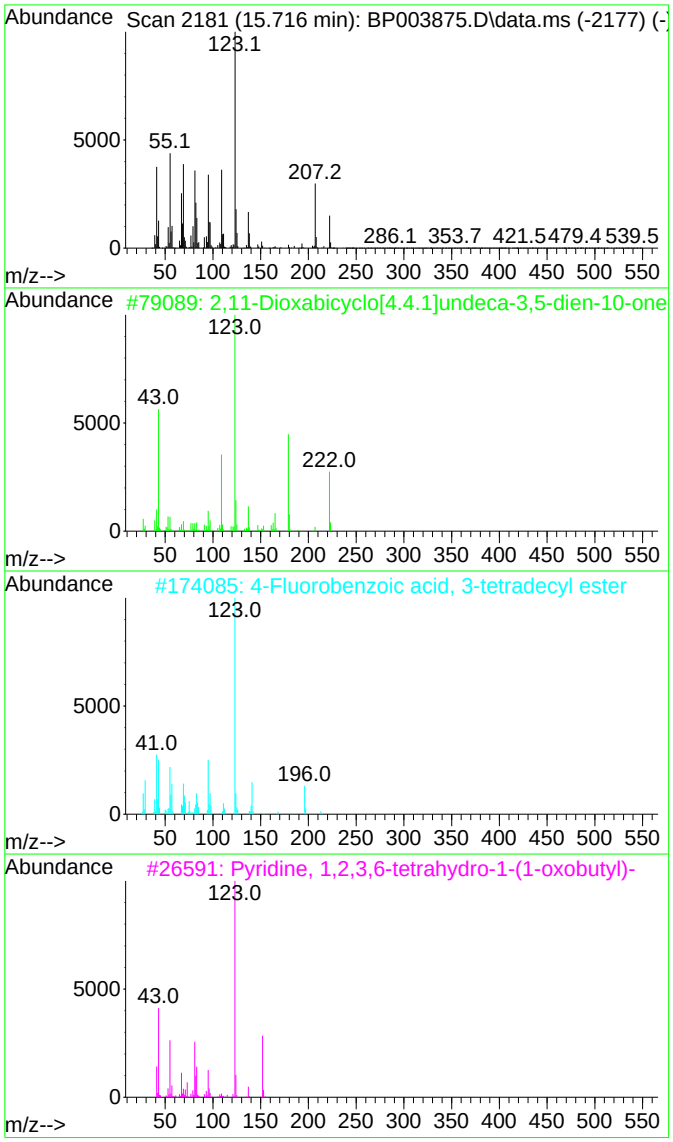
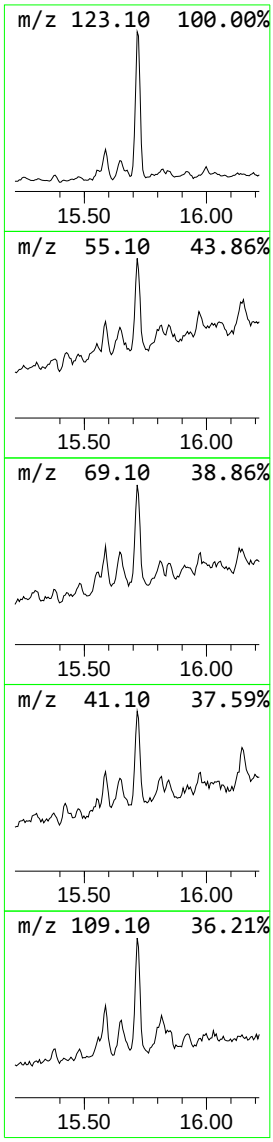
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 2,11-Dioxabicyclo[4.4.1]und... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.716	10.46 ng	1093490	Acenaphthene-d10	14.916

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,11-Dioxabicyclo[4.4.1]undeca-3...	222	C13H18O3	070412-52-1	53
2	4-Fluorobenzoic acid, 3-tetradec...	336	C21H33FO2	1000280-68-1	50
3	Pyridine, 1,2,3,6-tetrahydro-1-(...	153	C9H15NO	057150-46-6	50
4	4-Fluorobenzoic acid, 3-pentadec...	350	C22H35FO2	1000280-68-4	50
5	Diallyldivinylsilane	164	C10H16Si	119901-88-1	50





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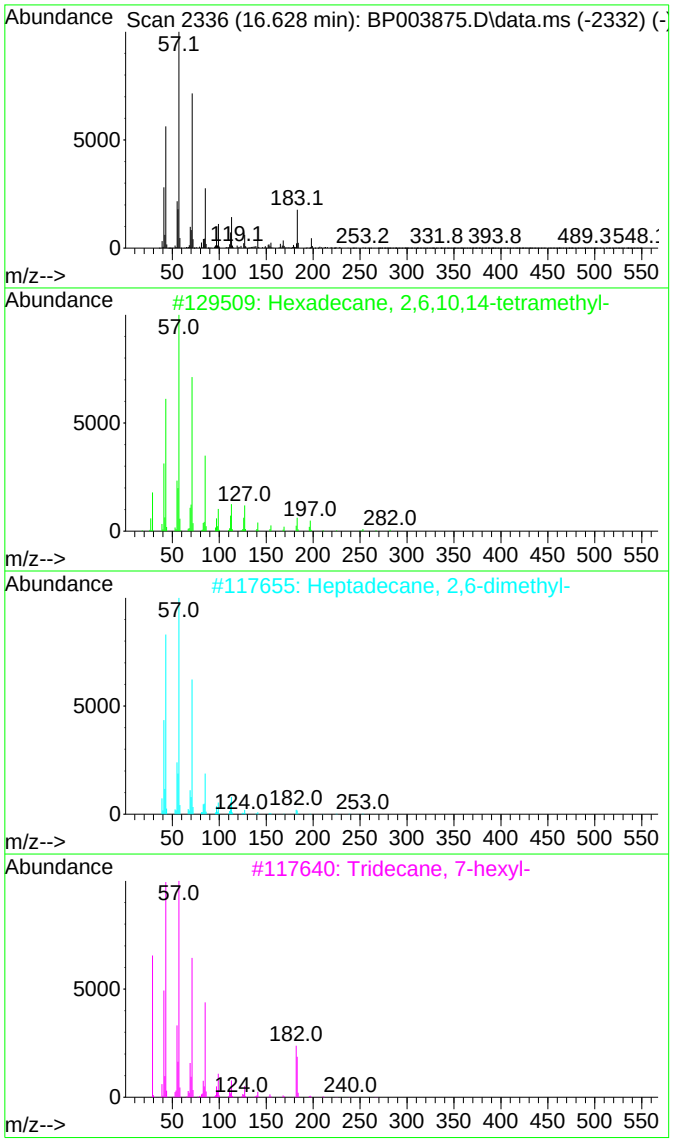
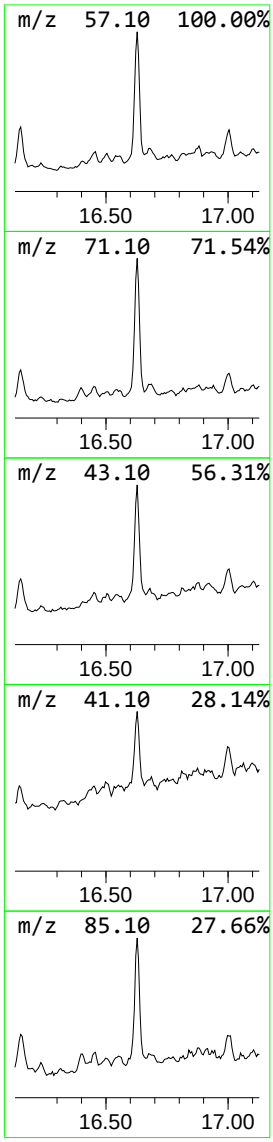
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 11 Hexadecane, 2,6,10,14-tetra... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.628	15.74 ng	1286610	Phenanthrene-d10	17.645

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane, 2,6,10,14-tetramethyl-	282	C20H42	000638-36-8	72
2	Heptadecane, 2,6-dimethyl-	268	C19H40	054105-67-8	70
3	Tridecane, 7-hexyl-	268	C19H40	007225-66-3	64
4	Dodecane, 2,7,10-trimethyl-	212	C15H32	074645-98-0	64
5	Heptane, 2,6-dimethyl-	128	C9H20	001072-05-5	62





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

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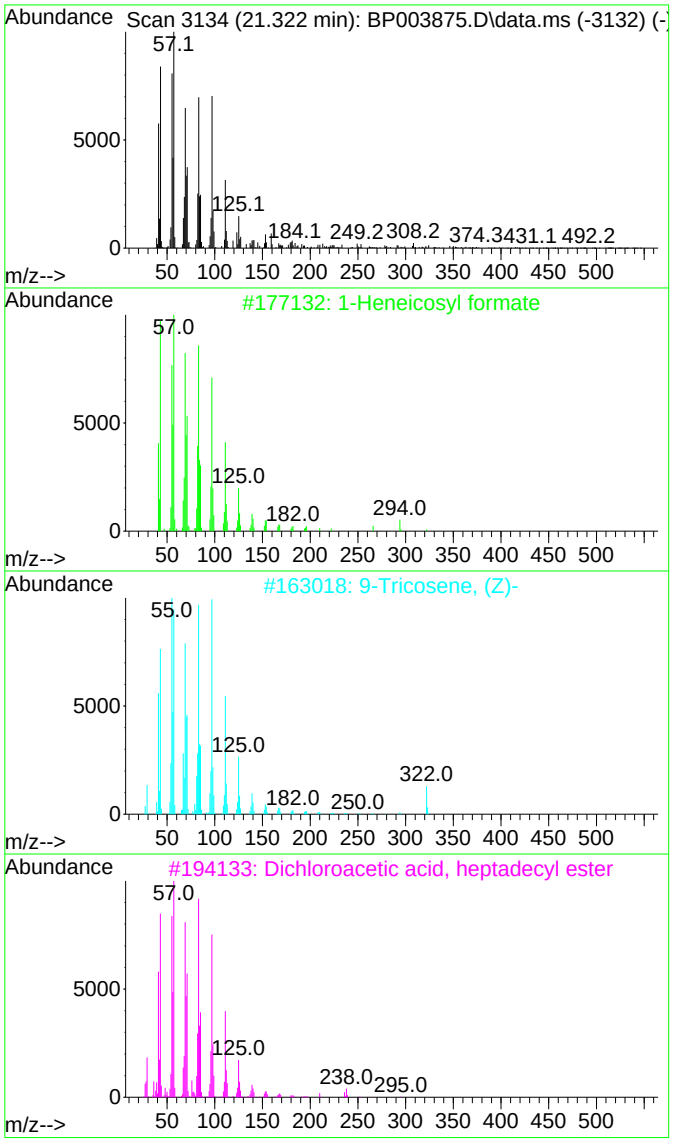
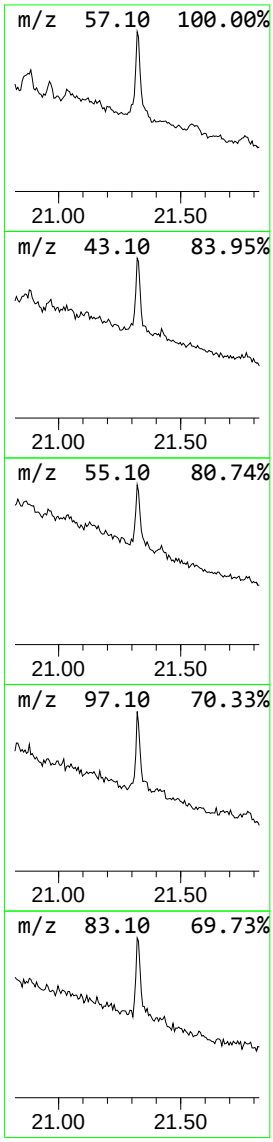
Peak Number 12 1-Heneicosyl formate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.322	10.39 ng	794567	Chrysene-d12	21.669

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosyl formate	340	C22H44O2	077899-03-7	96
2	9-Tricosene, (Z)-	322	C23H46	027519-02-4	95
3	Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	94
4	Heptafluorobutyric acid, n-tetra...	410	C18H29F7O2	007365-36-8	94
5	1-Docosene	308	C22H44	001599-67-3	94





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BNA_P
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TIC Library : C:\DATABASE\NIST11.L
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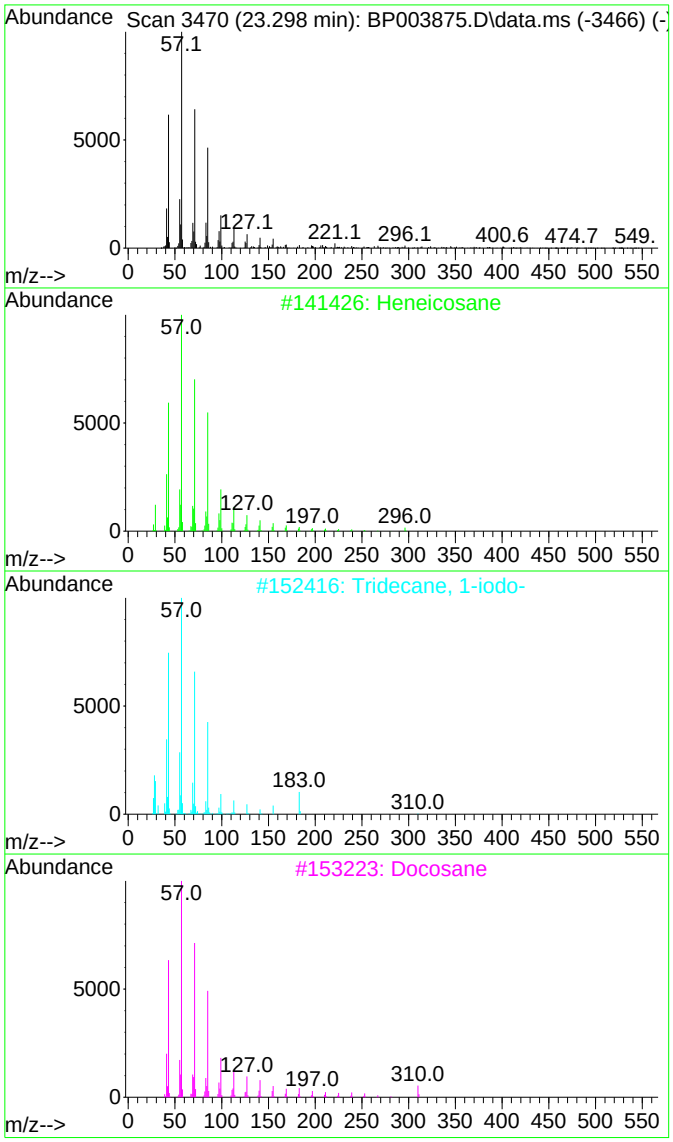
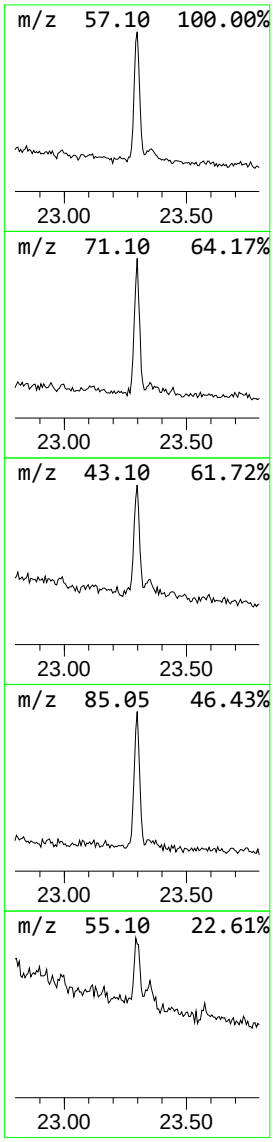
Peak Number 13 Heneicosane Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.298	2.56 ng	210295	Perylene-d12	24.151

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	98
2	Tridecane, 1-iodo-	310	C13H27I	035599-77-0	93
3	Docosane	310	C22H46	000629-97-0	93
4	Hexacosane	366	C26H54	000630-01-3	90
5	Tricosane	324	C23H48	000638-67-5	90





Tentatively Identified Compound (LSC) summary

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

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

TIC Top Hit name	RT	EstConc	Units	Response	Internal Standard #	RT	Resp	Conc
unknown2.946	2.946	136.8	ng	6392080	1	8.299	934806	20.0
Cyclohexane	3.105	4.7	ng	220728	1	8.299	934806	20.0
Butane, 2-metho...	3.193	8.2	ng	381834	1	8.299	934806	20.0
unknown14.475	14.475	2.0	ng	212208	3	14.916	2091330	20.0
unknown14.681	14.681	6.6	ng	690801	3	14.916	2091330	20.0
unknown14.763	14.763	10.2	ng	1066850	3	14.916	2091330	20.0
Cyclohexene, 1,...	15.022	3.3	ng	347108	3	14.916	2091330	20.0
unknown15.428	15.428	3.3	ng	342926	3	14.916	2091330	20.0
unknown15.586	15.586	3.3	ng	346220	3	14.916	2091330	20.0
2,11-Dioxabicyc...	15.716	10.5	ng	1093490	3	14.916	2091330	20.0
Hexadecane, 2,6...	16.628	15.7	ng	1286610	4	17.645	1634500	20.0
1-Heneicosyl fo...	21.322	10.4	ng	794567	5	21.669	1528920	20.0
Heneicosane	23.298	2.6	ng	210295	6	24.151	1645910	20.0