LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF060923\
Data File : BF133677.D
Acq On : 09 Jun 2023 15:47
Operator : CG\JU
Sample : 03064-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CHRT-24236

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-BF060923.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF133677.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.051	496	504	511	rBV	51452	64947	3.16%	0.335%
2	5.451	567	572	575	rBV	1727654	1666041	81.01%	8.582%
3	6.463	739	744	747	rBV	1840673	1824299	88.71%	9.398%
4	6.833	804	807	811	rBV	833452	647837	31.50%	3.337%
5	7.398	898	903	906	rBV	1389479	1216538	59.15%	6.267%
6	8.122	1022	1026	1029	rBV	927929	821320	39.94%	4.231%
7	9.139	1196	1199	1203	rVB4	45116	39124	1.90%	0.202%
8	9.198	1204	1209	1212	rBV	2404802	2056590	100.00%	10.594%
9	9.274	1218	1222	1225	rBV3	101612	127626	6.21%	0.657%
10	9.469	1253	1255	1257	rBV2	46390	45264	2.20%	0.233%
11	9.580	1272	1274	1276	rBV	210173	220048	10.70%	1.134%
12	9.627	1279	1282	1288	rVV7	124859	255420	12.42%	1.316%
13	9.745	1298	1302	1304	rBV4	204881	264720	12.87%	1.364%
14	9.786	1306	1309	1312	rVB2	357033	351994	17.12%	1.813%
15	9.874	1319	1324	1327	rVB	993072	1063684	51.72%	5.479%
16	10.139	1366	1369	1371	rBV3	158958	189630	9.22%	0.977%
17	10.286	1391	1394	1396	rBV3	431620	394580	19.19%	2.033%
18	10.533	1434	1436	1440	rVB	315235	300277	14.60%	1.547%
19	10.668	1456	1459	1462	rBV	1052183	1022072	49.70%	5.265%
20	10.804	1479	1482	1489	rVB	1175128	1293604	62.90%	6.664%
21	11.274	1559	1562	1567	rVB	1181016	1139685	55.42%	5.871%
22	11.374	1577	1579	1584	rBV	680743	705433	34.30%	3.634%
23	12.962	1846	1849	1853	rVB	1614683	1497370	72.81%	7.713%
24	14.015	2024	2028	2030	rVB	599926	574301	27.92%	2.958%
25	14.480	2105	2107	2111	rBV3	45990	56964	2.77%	0.293%
26	14.521	2112	2114	2125	rVB5	73343	171954	8.36%	0.886%
27	15.045	2201	2203	2212	rVB	42479	74365	3.62%	0.383%
28	15.127	2213	2217	2220	rVV	224064	225619	10.97%	1.162%
29	15.409	2262	2265	2268	rVB	57154	56446	2.74%	0.291%
30	15.474	2271	2276	2280	rBV	481265	595511	28.96%	3.068%
31	15.709	2312	2316	2319	rBV3	50348	73717	3.58%	0.380%
32	15.945	2351	2356	2361	rVB	137560	202975	9.87%	1.046%
33	16.739	2488	2491	2502	rVB4	55170	126800	6.17%	0.653%
34	17.374	2595	2599	2605	rVB3	20631	45787	2.23%	0.236%

Sum of corrected areas: 19412542

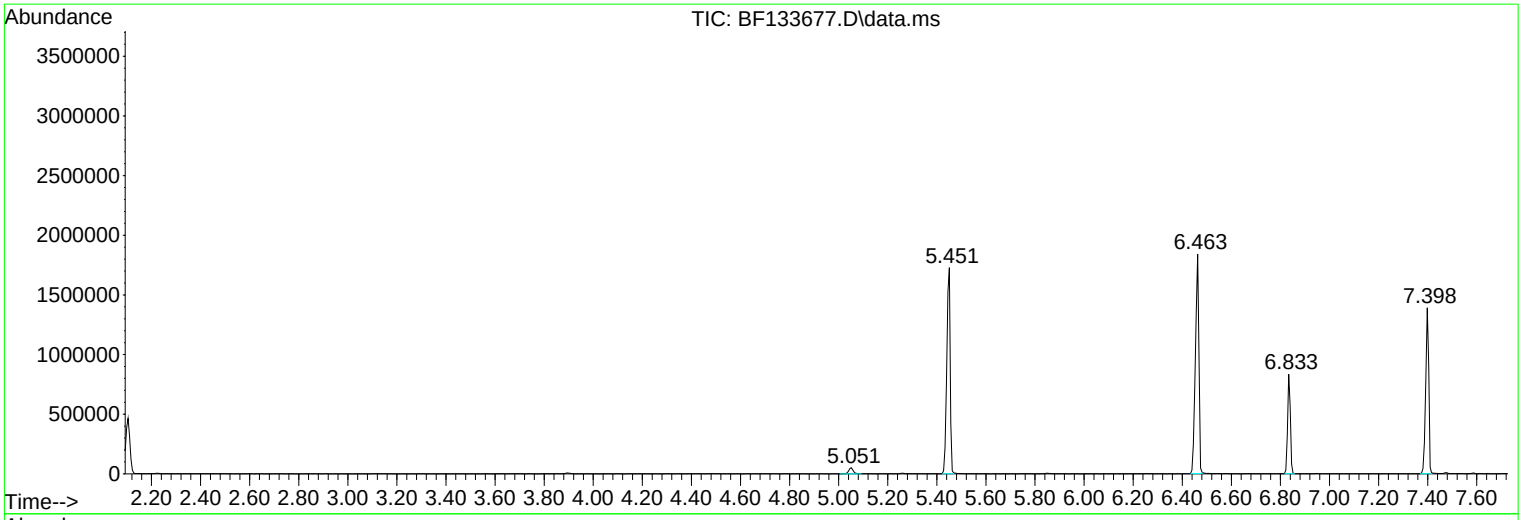
Instrument :
BNA_F
ClientSampleId :
CHRT-24236

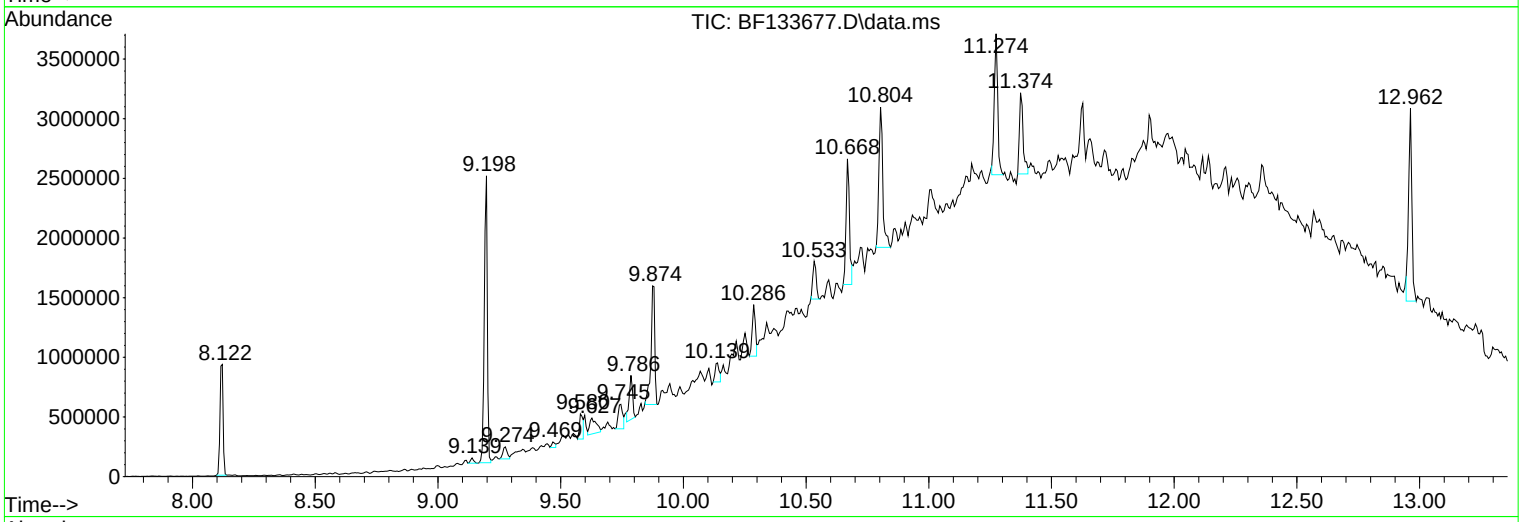
Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF060923\
Data File : BF133677.D
Acq On : 09 Jun 2023 15:47
Operator : CG\JU
Sample : 03064-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

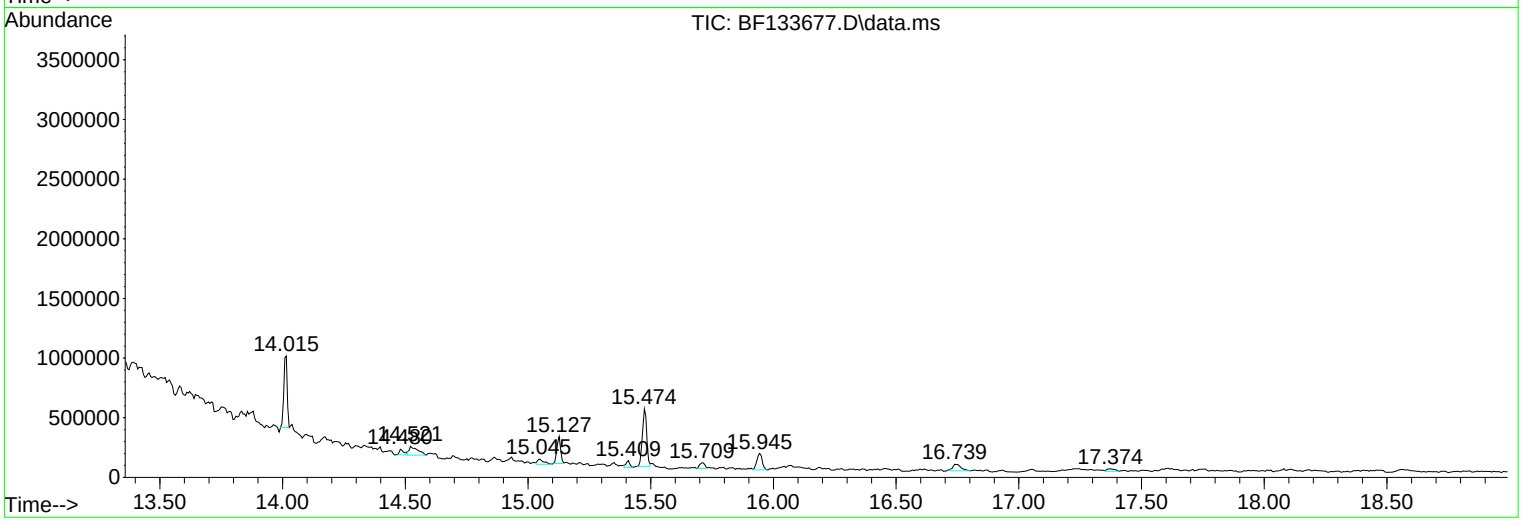
Instrument :
BNA_F
ClientSampleId :
CHRT-24236

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P







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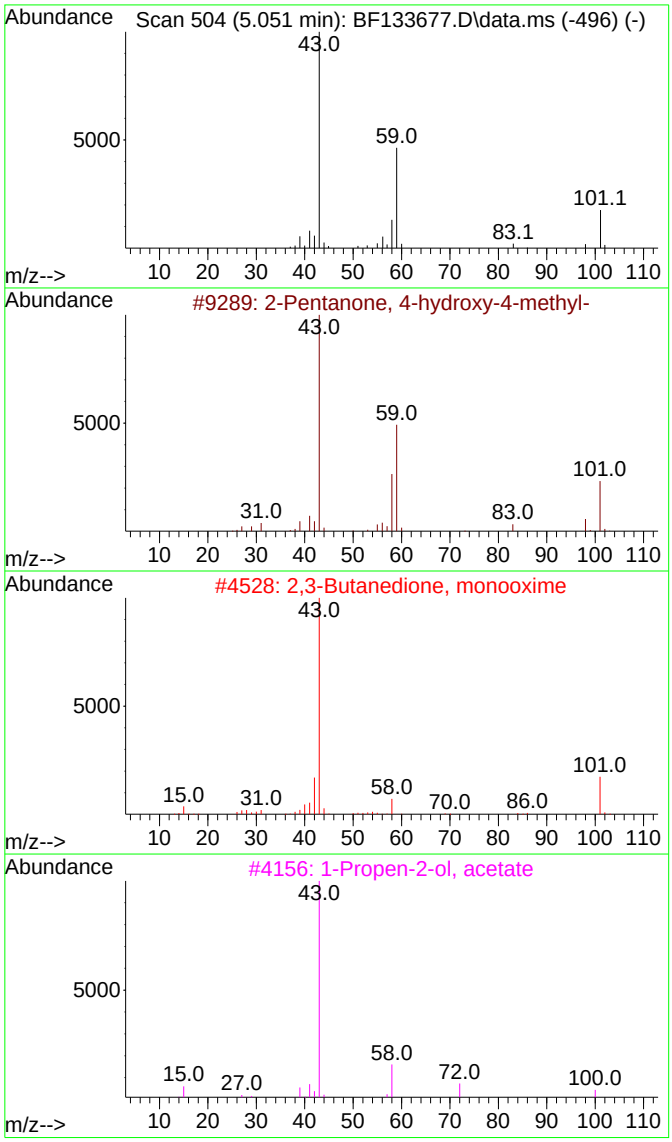
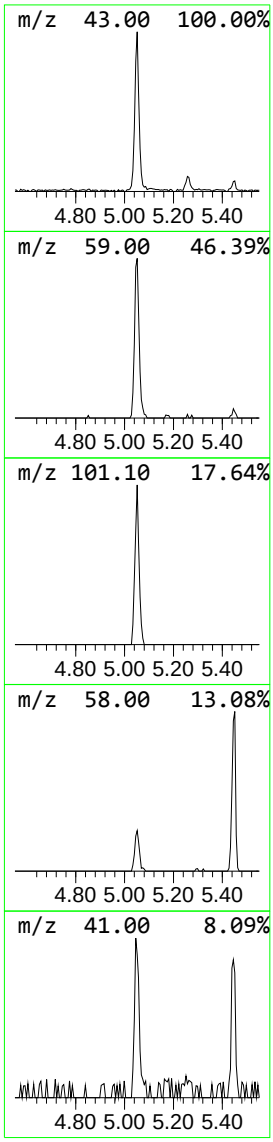
****
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.051	2.01 ng	64947	1,4-Dichlorobenzene-d4	6.833

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	27
3	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12
4	Acetamide, N-(cyanomethyl)-	98	C4H6N2O	004814-80-6	9
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9





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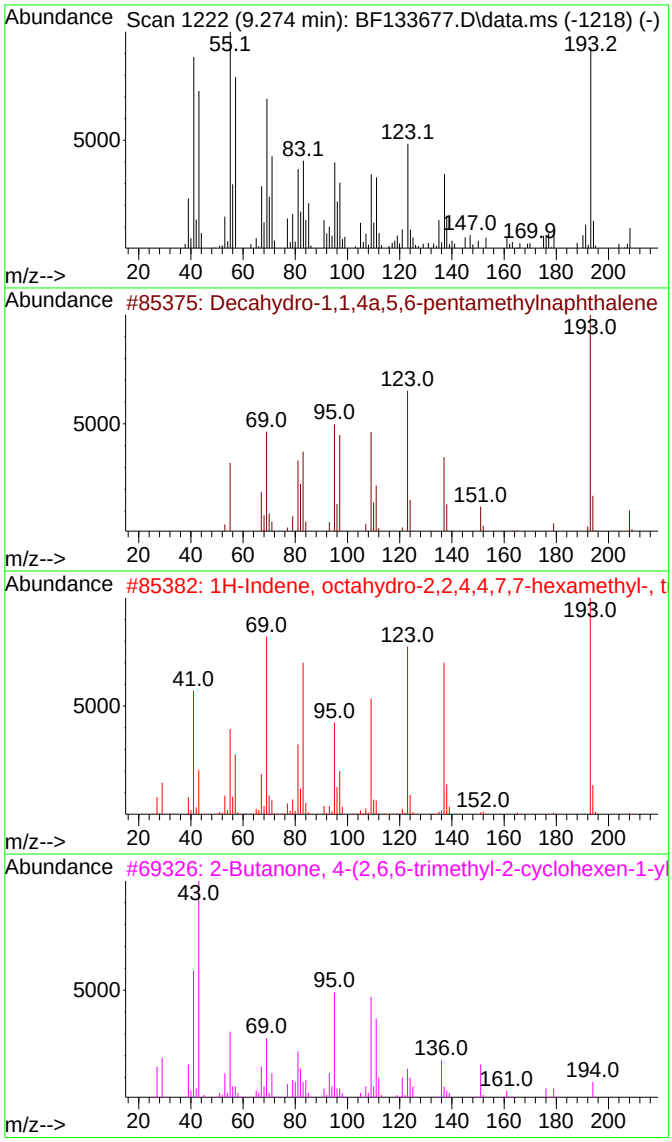
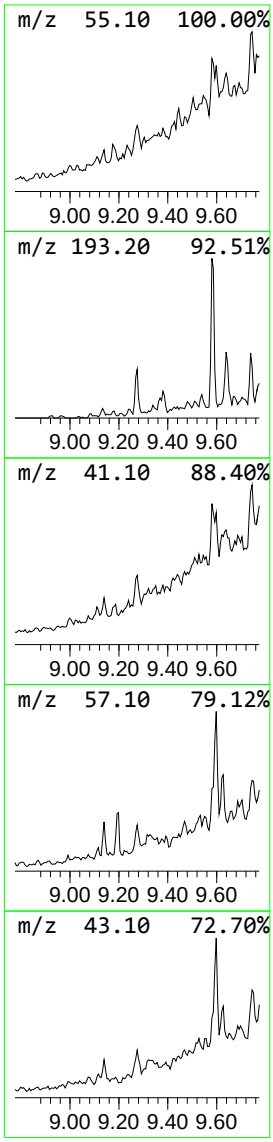
****
Peak Number 2 Decahydro-1,1,4a,5,6-pentam... Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.274	2.40 ng	127626	Acenaphthene-d10	9.880

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Decahydro-1,1,4a,5,6-pentamethyl...	208	C15H28	080655-44-3	95
2	1H-Indene, octahydro-2,2,4,4,7,7...	208	C15H28	054832-83-6	59
3	2-Butanone, 4-(2,6,6-trimethyl-2...	194	C13H22O	039721-65-8	38
4	Acridine, 9-methyl-	193	C14H11N	000611-64-3	38
5	4-Amino-N-hydroxypyrazolo[3,2-c]...	193	C6H7N7O	1000443-50-2	38





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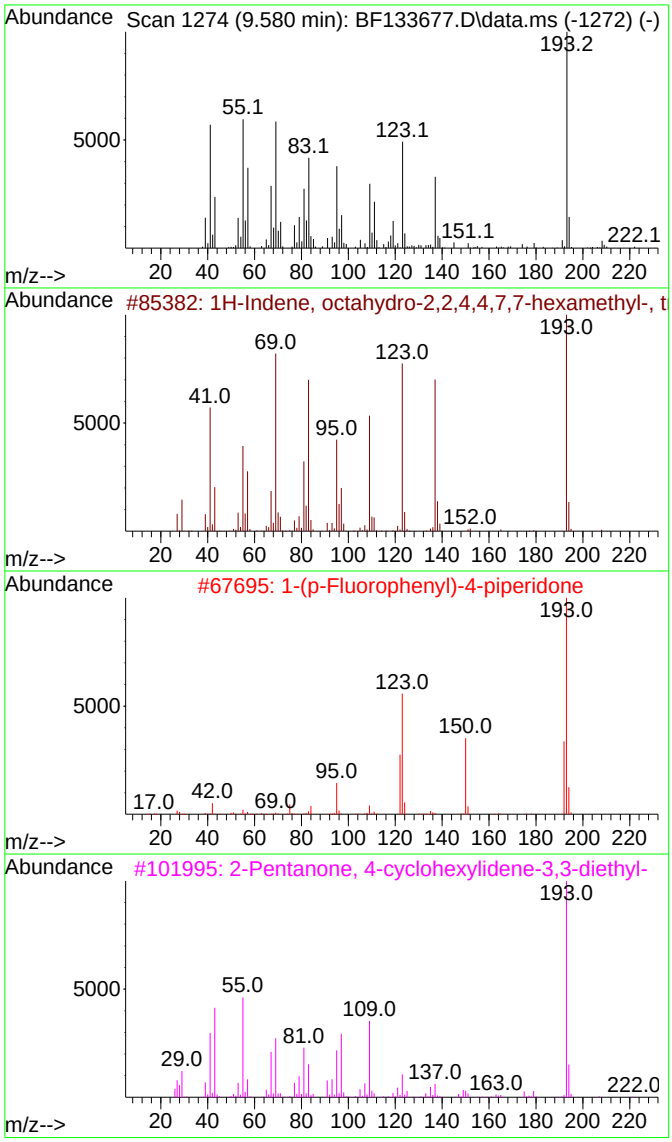
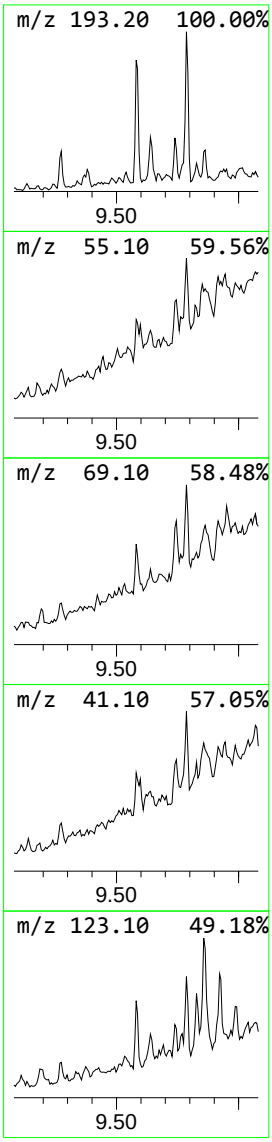
****
Peak Number 3 1H-Indene, octahydro-2,2,4,... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.580	4.14 ng	220048	Acenaphthene-d10	9.880

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Indene, octahydro-2,2,4,4,7,7...	208	C15H28	054832-83-6	59
2	1-(p-Fluorophenyl)-4-piperidone	193	C11H12FNO	1000238-56-7	47
3	2-Pentanone, 4-cyclohexylidene-3...	222	C15H26O	313253-65-5	32
4	Butan-2-one, 1-[3-(3,3-dimethyl-...	278	C16H26N2O2	1000303-34-2	27
5	2H-Spiro[1-benzofuran-3,2'-[1,3]...	193	C10H11NO3	1000387-33-4	25





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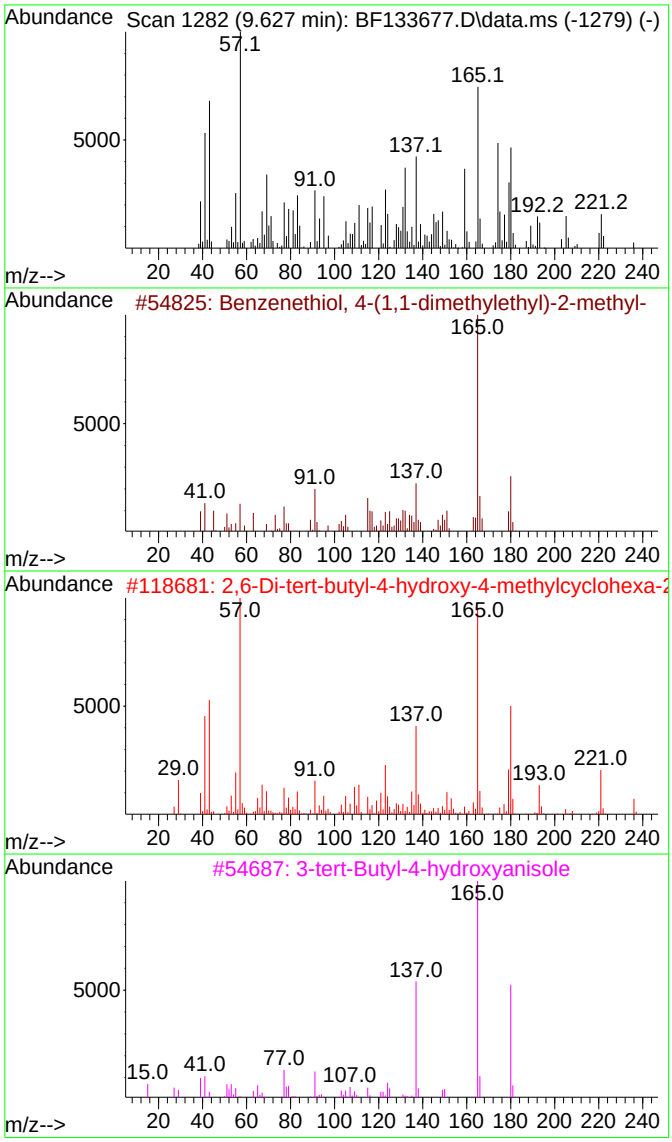
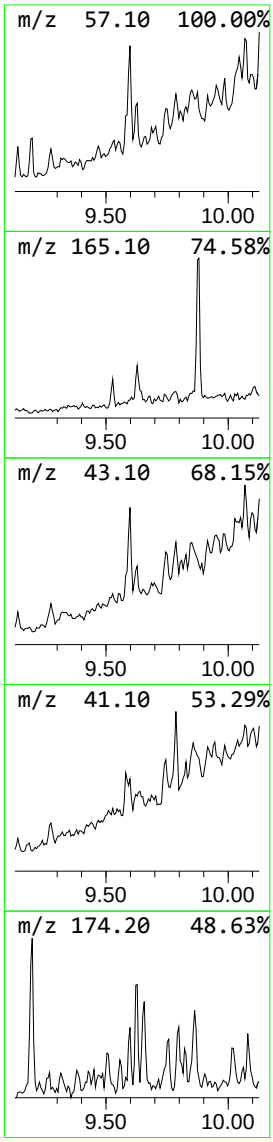
****

Peak Number 4 unknown9.627 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.627	4.80 ng	255420	Acenaphthene-d10	9.880

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzenethiol, 4-(1,1-dimethyleth...	180	C11H16S	015570-10-2	47
2	2,6-Di-tert-butyl-4-hydroxy-4-me...	236	C15H24O2	010396-80-2	46
3	3-tert-Butyl-4-hydroxyanisole	180	C11H16O2	000121-00-6	45
4	Phenol, 3-(1,1-dimethylethyl)-4-...	180	C11H16O2	000088-32-4	45
5	9H-Fluorene, 2-methyl-	180	C14H12	001430-97-3	38





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TIC Library : C:\Database\NIST20.L
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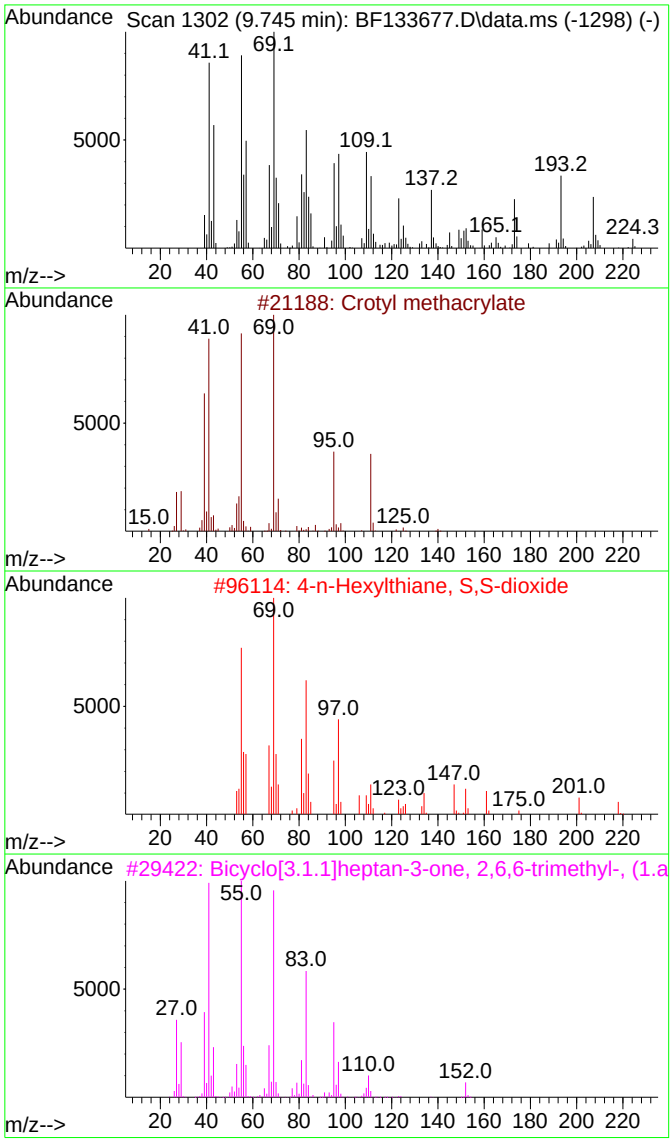
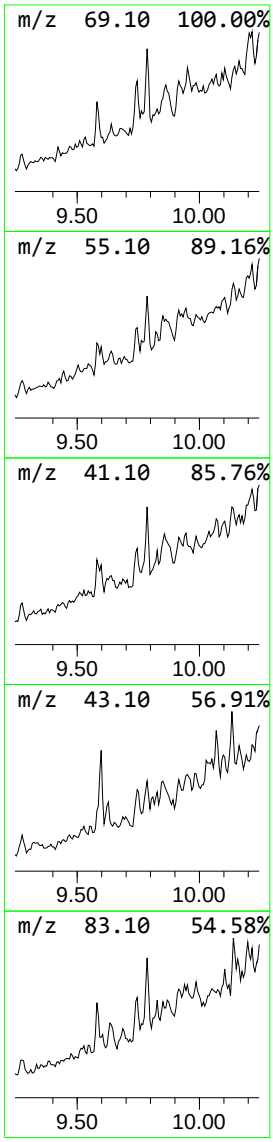
****

Peak Number 5 unknown9.745 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.745	4.98 ng	264720	Acenaphthene-d10	9.880

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Crotyl methacrylate	140	C8H12O2	007376-45-6	46
2	4-n-Hexylthiane, S,S-dioxide	218	C11H22O2S	070928-52-8	38
3	Bicyclo[3.1.1]heptan-3-one, 2,6,...	152	C10H16O	015358-88-0	30
4	Nonane, 1,9-dibromo-	284	C9H18Br2	004549-33-1	25
5	Dichloroacetic acid, 4-hexadecyl...	352	C18H34Cl2O2	1000282-98-1	15





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BNA_F
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TIC Library : C:\Database\NIST20.L
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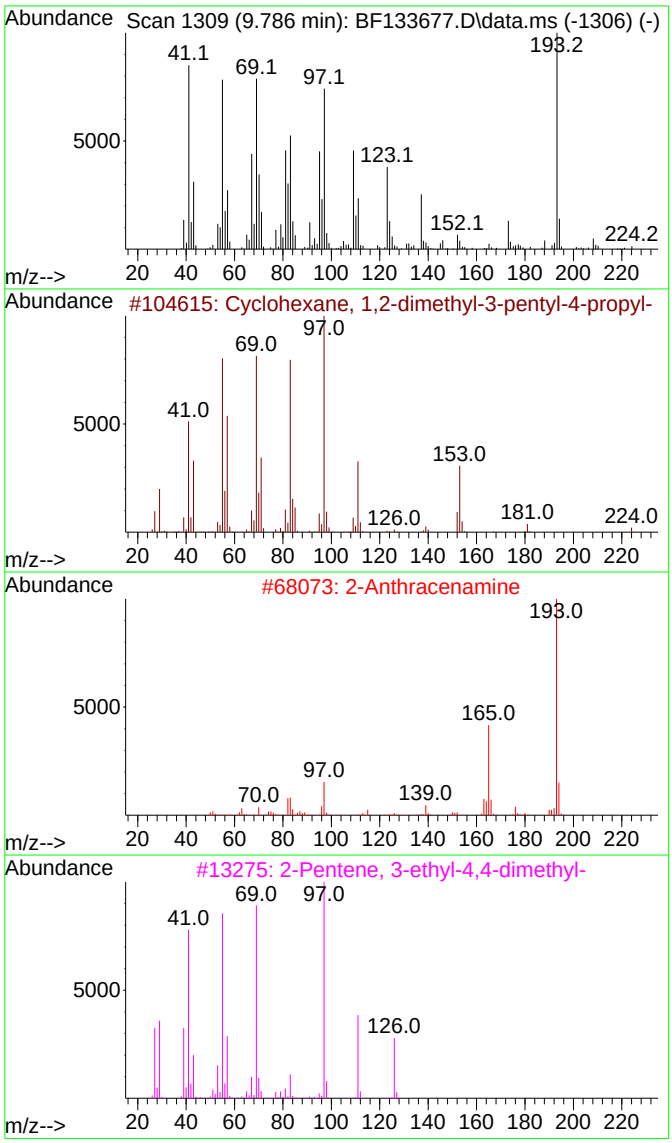
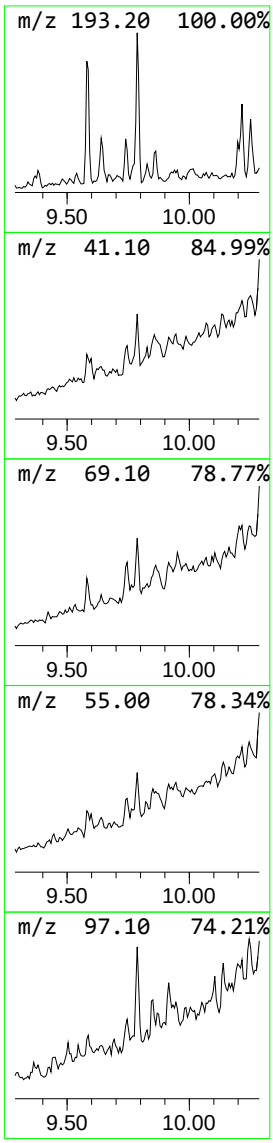
****
Peak Number 6 Cyclohexane, 1,2-dimethyl-3... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.786	6.62 ng	351994	Acenaphthene-d10	9.880

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexane, 1,2-dimethyl-3-pent...	224	C16H32	062376-17-4	53
2	2-Anthracenamine	193	C14H11N	000613-13-8	46
3	2-Pentene, 3-ethyl-4,4-dimethyl-	126	C9H18	053907-59-8	27
4	Cyclopropane, 1,1-dimethyl-2-(2-...	124	C9H16	069147-03-1	18
5	Cyclohexane, 1-(cyclohexylmethyl...	194	C14H26	054823-98-2	11





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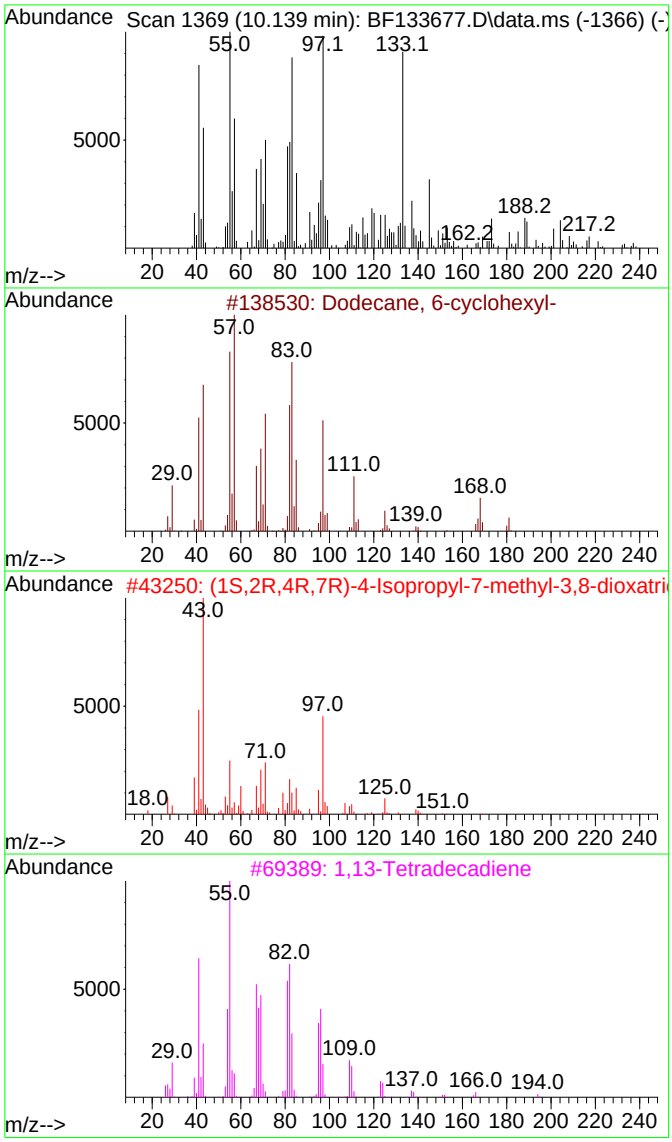
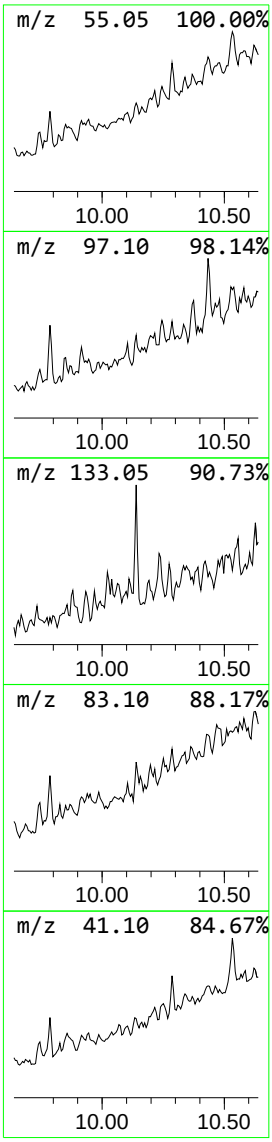
****

Peak Number 7 unknown10.139 Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.139	3.57 ng	189630	Acenaphthene-d10	9.880

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dodecane, 6-cyclohexyl-	252	C18H36	013151-86-5	38
2	(1S,2R,4R,7R)-4-Isopropyl-7-meth...	168	C10H16O2	001619-26-7	35
3	1,13-Tetradecadiene	194	C14H26	021964-49-8	25
4	Cyclohexane, 1,3-dimethyl-, cis-	112	C8H16	000638-04-0	15
5	2-Furanmethanol, .alpha.-(2-nitr...	185	C8H11NO4	103077-75-4	15





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TIC Library : C:\Database\NIST20.L
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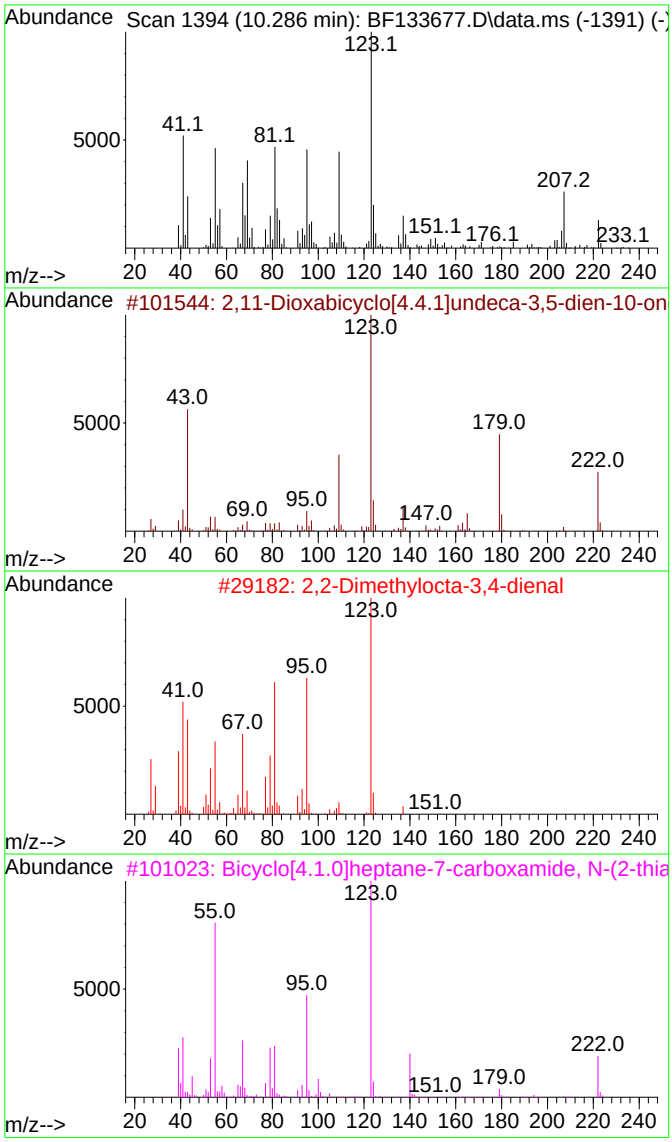
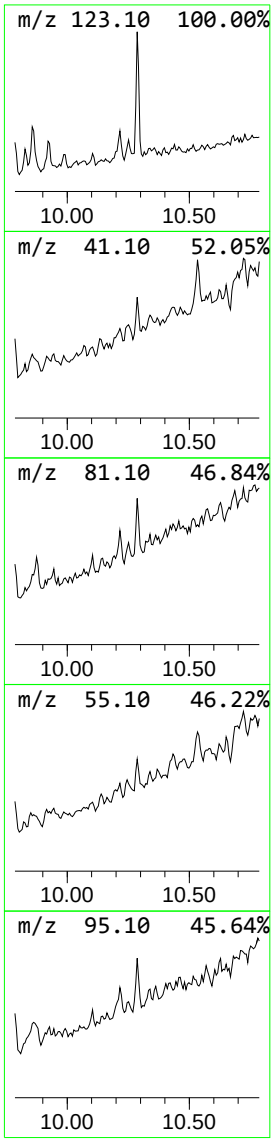
****
Peak Number 8 2,11-Dioxabicyclo[4.4.1]und... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.286	7.42 ng	394580	Acenaphthene-d10	9.880

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,11-Dioxabicyclo[4.4.1]undeca-3...	222	C13H18O3	070412-52-1	50
2	2,2-Dimethylocta-3,4-dienal	152	C10H16O	000590-71-6	43
3	Bicyclo[4.1.0]heptane-7-carboxam...	222	C11H14N2OS	329912-72-3	43
4	Methyl 2-fluorobenzoate	154	C8H7FO2	000394-35-4	43
5	1-(4-Hydroxyphenyl)propane-1,2-d...	168	C9H12O3	1000495-85-4	38





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ClientSampleId :
CHRT-24236

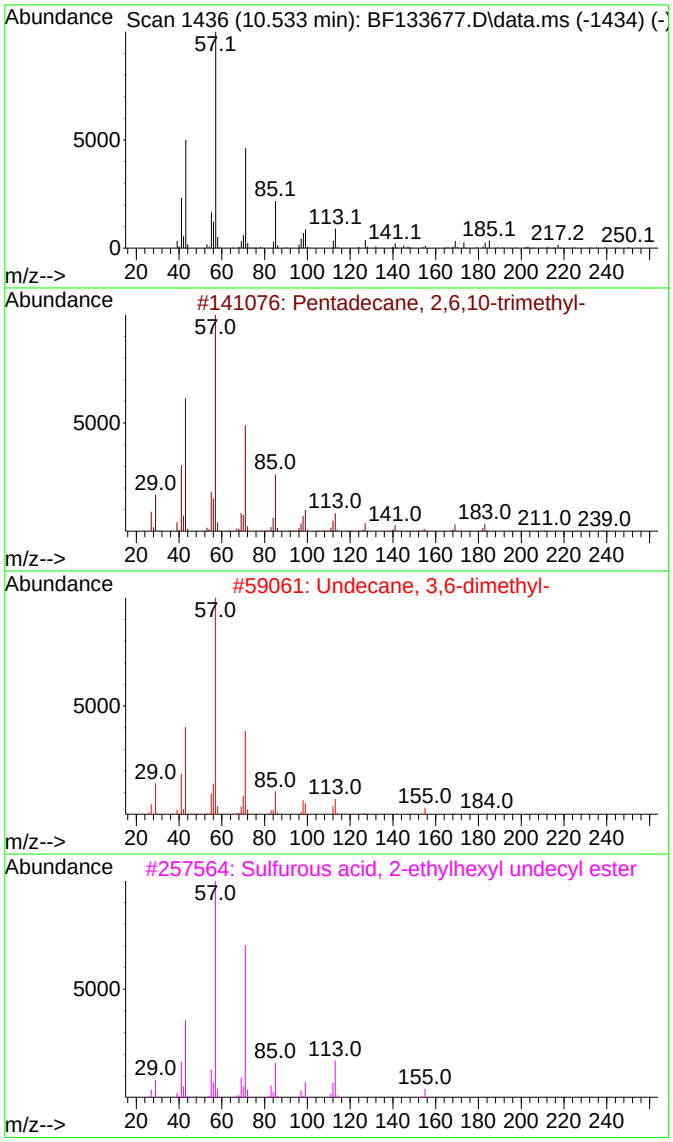
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

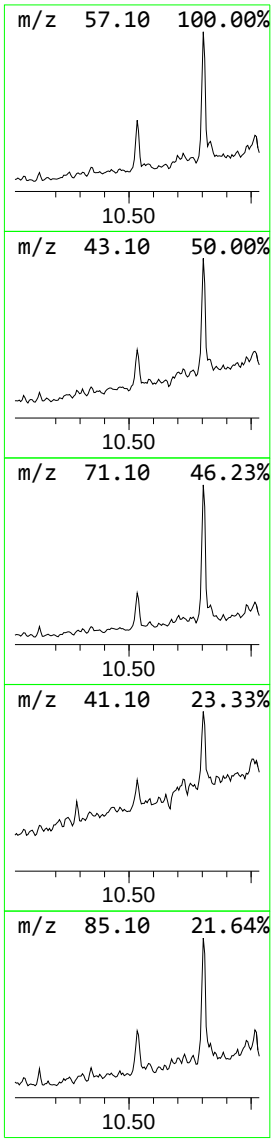
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 Pentadecane, 2,6,10-trimethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.533	5.65 ng	300277	Acenaphthene-d10	9.880

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecane, 2,6,10-trimethyl-	254	C18H38	003892-00-0	86
2	Undecane, 3,6-dimethyl-	184	C13H28	017301-28-9	64
3	Sulfurous acid, 2-ethylhexyl und...	348	C19H40O3S	1000309-19-4	53
4	Undecane, 4,6-dimethyl-	184	C13H28	017312-82-2	52
5	Sulfurous acid, dodecyl 2-ethylh...	362	C20H42O3S	1000309-19-5	50





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Acq On : 09 Jun 2023 15:47
Operator : CG\JU
Sample : 03064-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CHRT-24236

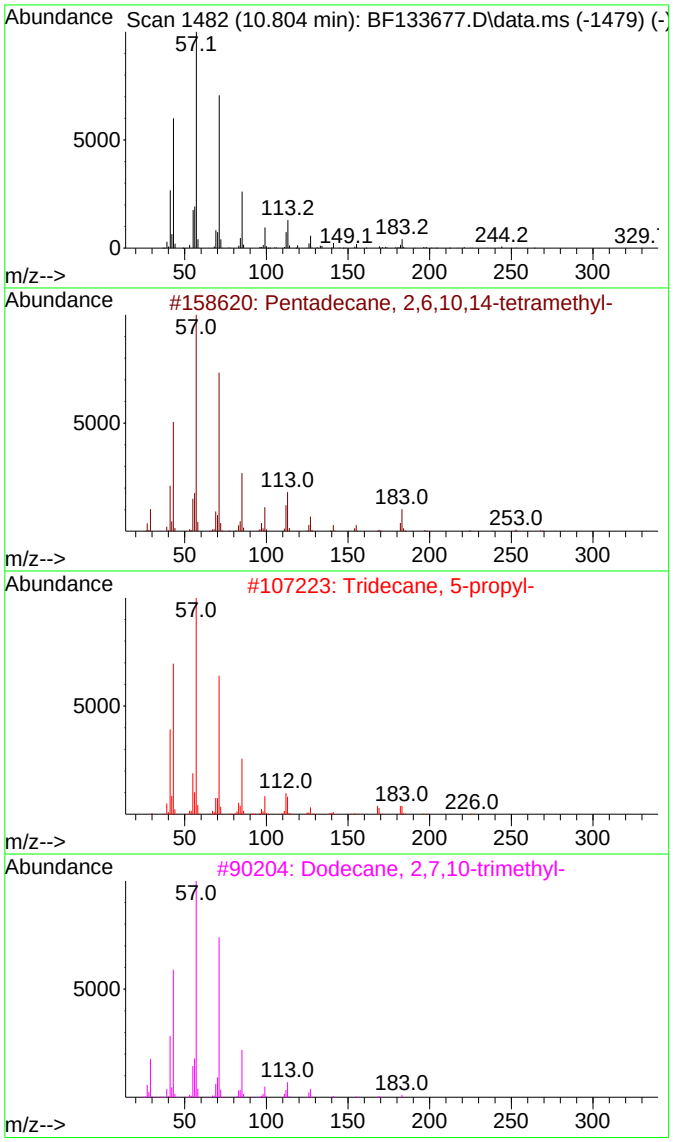
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

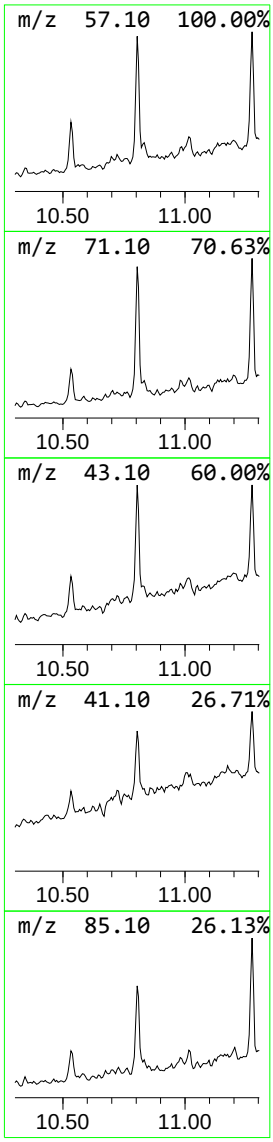
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 Pentadecane, 2,6,10,14-tetr... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.804	36.68 ng	1293600	Phenanthrene-d10	11.374

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecane, 2,6,10,14-tetramethyl-	268	C19H40	001921-70-6	90
2	Tridecane, 5-propyl-	226	C16H34	055045-11-9	87
3	Dodecane, 2,7,10-trimethyl-	212	C15H32	074645-98-0	80
4	Dodecane, 4,6-dimethyl-	198	C14H30	061141-72-8	74
5	Nonane, 3,7-dimethyl-	156	C11H24	017302-32-8	62





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Instrument :
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ClientSampleId :
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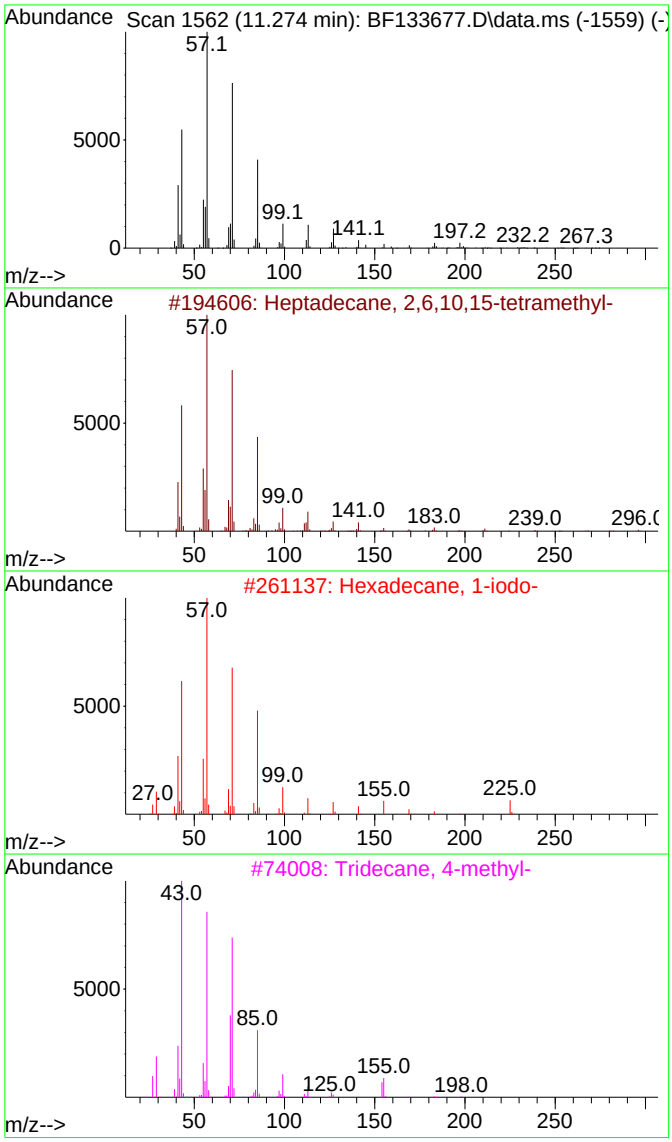
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

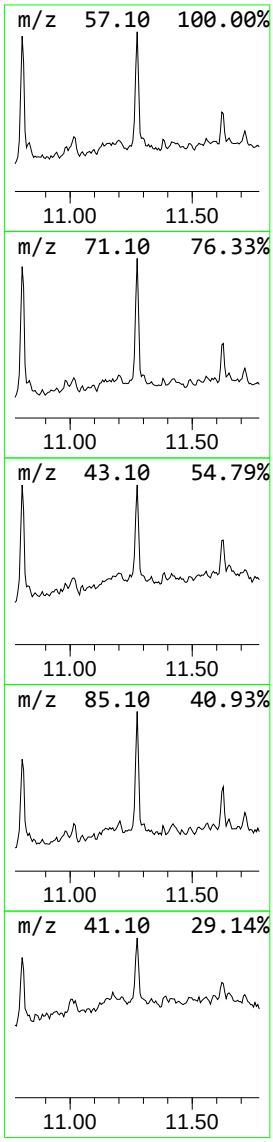
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 11 Heptadecane, 2,6,10,15-tetr... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.274	32.31 ng	1139690	Phenanthrene-d10	11.374

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	90
2	Hexadecane, 1-iodo-	352	C16H33I	000544-77-4	86
3	Tridecane, 4-methyl-	198	C14H30	026730-12-1	81
4	Tetradecane, 1-iodo-	324	C14H29I	019218-94-1	80
5	Dodecane, 2,6,10-trimethyl-	212	C15H32	003891-98-3	80





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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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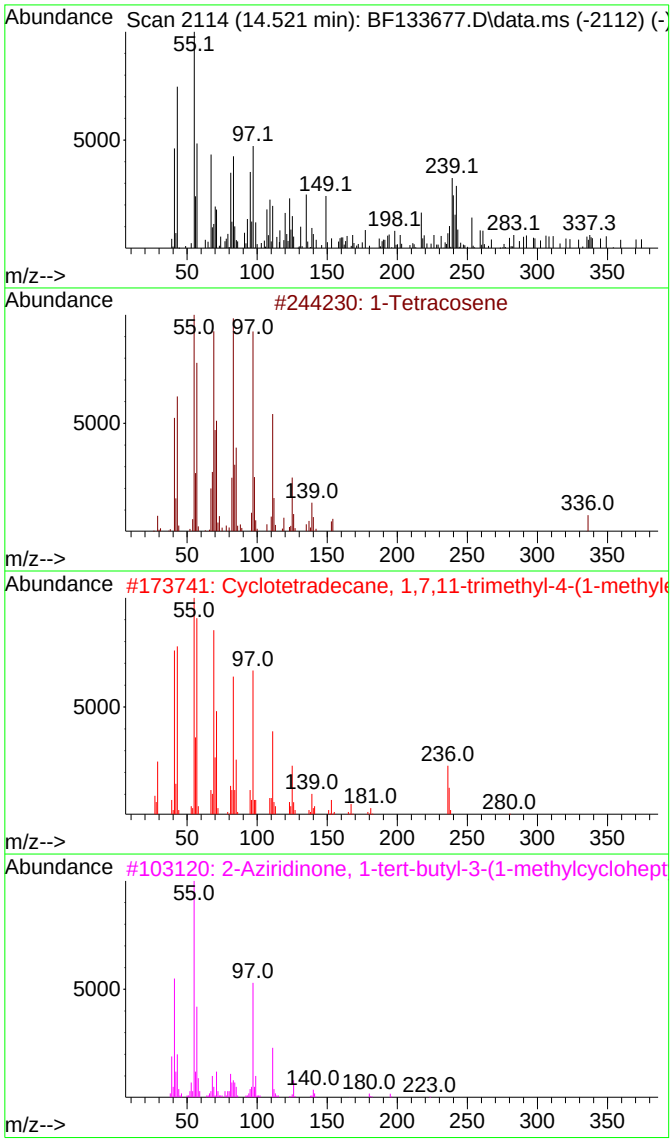
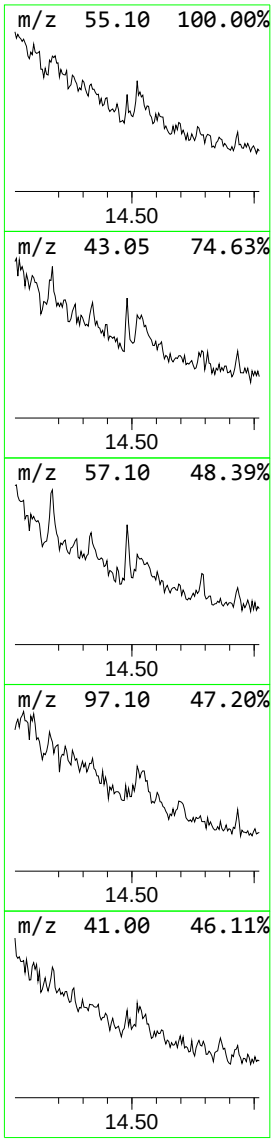
Peak Number 12 unknown14.521 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.521	5.99 ng	171954	Chrysene-d12	14.015

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Tetracosene	336	C24H48	010192-32-2	25
2	Cyclotetradecane, 1,7,11-trimeth...	280	C20H40	001786-12-5	22
3	2-Aziridinone, 1-tert-butyl-3-(1...	223	C14H25NO	026944-18-3	14
4	5-Isopropyl-6-methyl-hepta-3,5-d...	168	C11H20O	1010187-77-8	14
5	1-Decene	140	C10H20	000872-05-9	14





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ALS Vial : 5 Sample Multiplier: 1

Instrument :
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ClientSampleId :
CHRT-24236

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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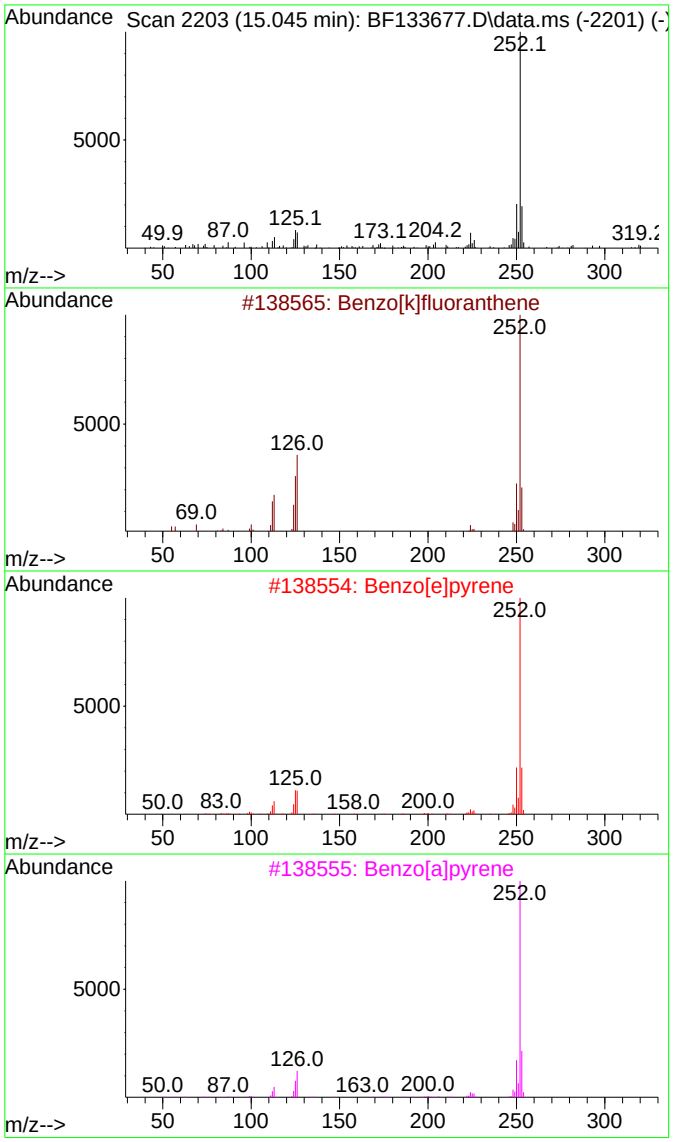
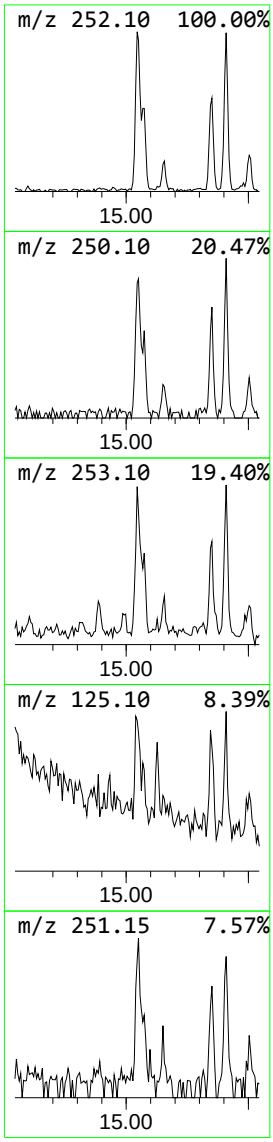
Peak Number 13 Benzo[e]pyrene Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.045	2.50 ng	74365	Perylene-d12	15.474

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[k]fluoranthene	252	C20H12	000207-08-9	90
2	Benzo[e]pyrene	252	C20H12	000192-97-2	90
3	Benzo[a]pyrene	252	C20H12	000050-32-8	90
4	Benzo[j]fluoranthene	252	C20H12	000205-82-3	89
5	Benzo[b]fluoranthene	252	C20H12	000205-99-2	81





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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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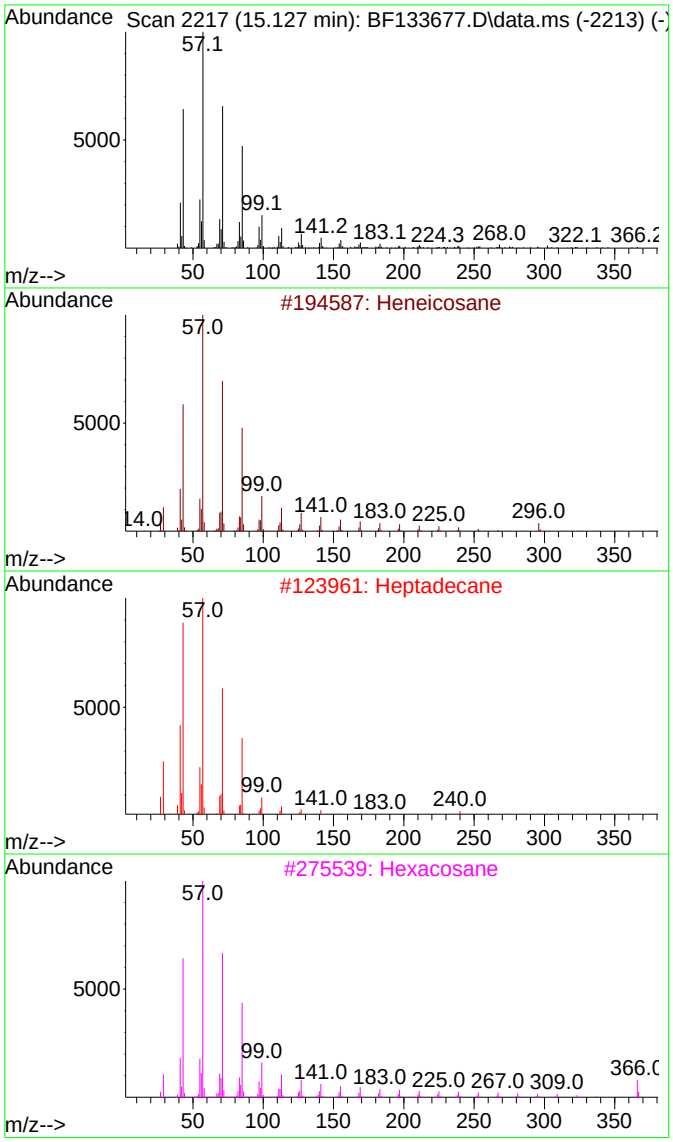
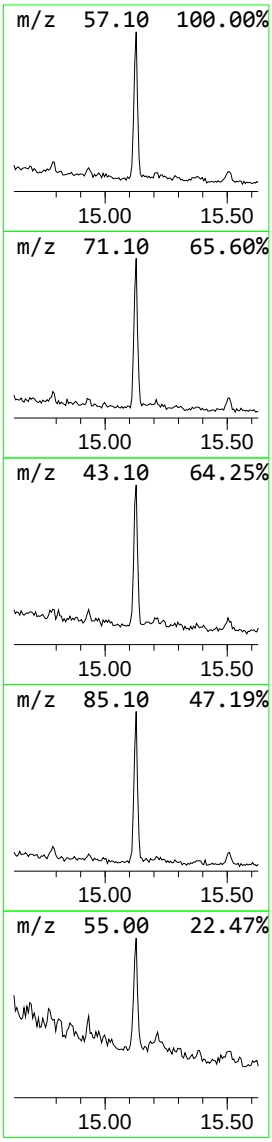
Peak Number 14 Heneicosane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.127	7.58 ng	225619	Perylene-d12	15.474

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	97
2	Heptadecane	240	C17H36	000629-78-7	94
3	Hexacosane	366	C26H54	000630-01-3	93
4	Nonadecane	268	C19H40	000629-92-5	93
5	Docosane	310	C22H46	000629-97-0	91





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ALS Vial : 5 Sample Multiplier: 1

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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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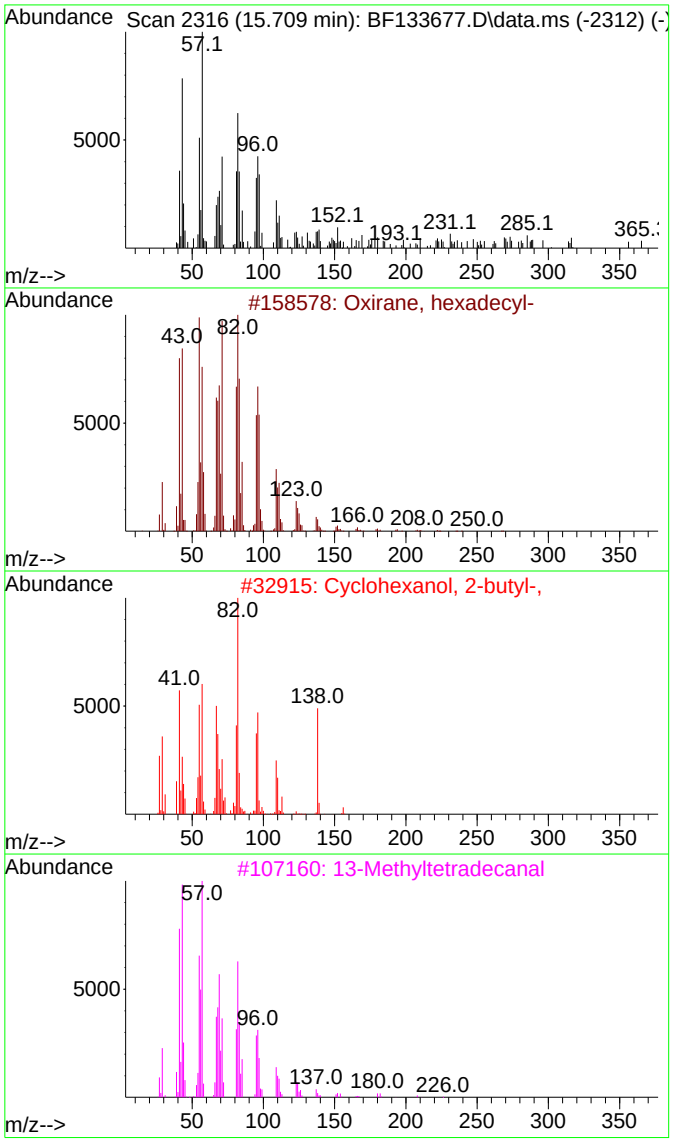
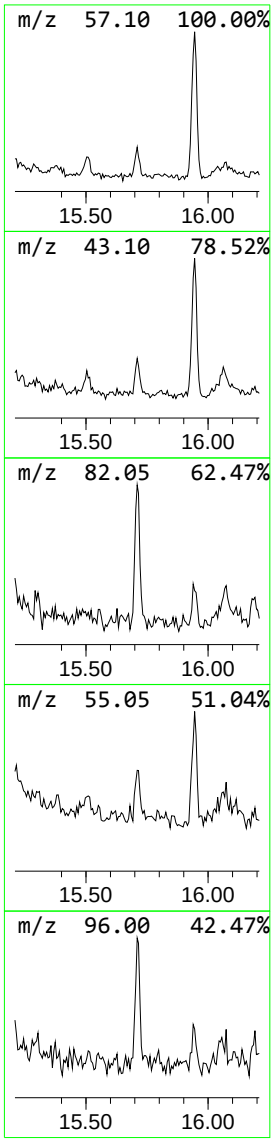
Peak Number 15 Oxirane, hexadecyl- Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.709	2.48 ng	73717	Perylene-d12	15.474

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oxirane, hexadecyl-	268	C18H36O	007390-81-0	87
2	Cyclohexanol, 2-butyl-,	156	C10H20O	036159-49-6	64
3	13-Methyltetradecanal	226	C15H30O	075853-51-9	64
4	14-Heptadecenal	252	C17H32O	1010144-58-0	62
5	7-Hexadecen-1-ol, acetate, (Z)-	282	C18H34O2	023192-42-9	53





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Sample : 03064-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CHRT-24236

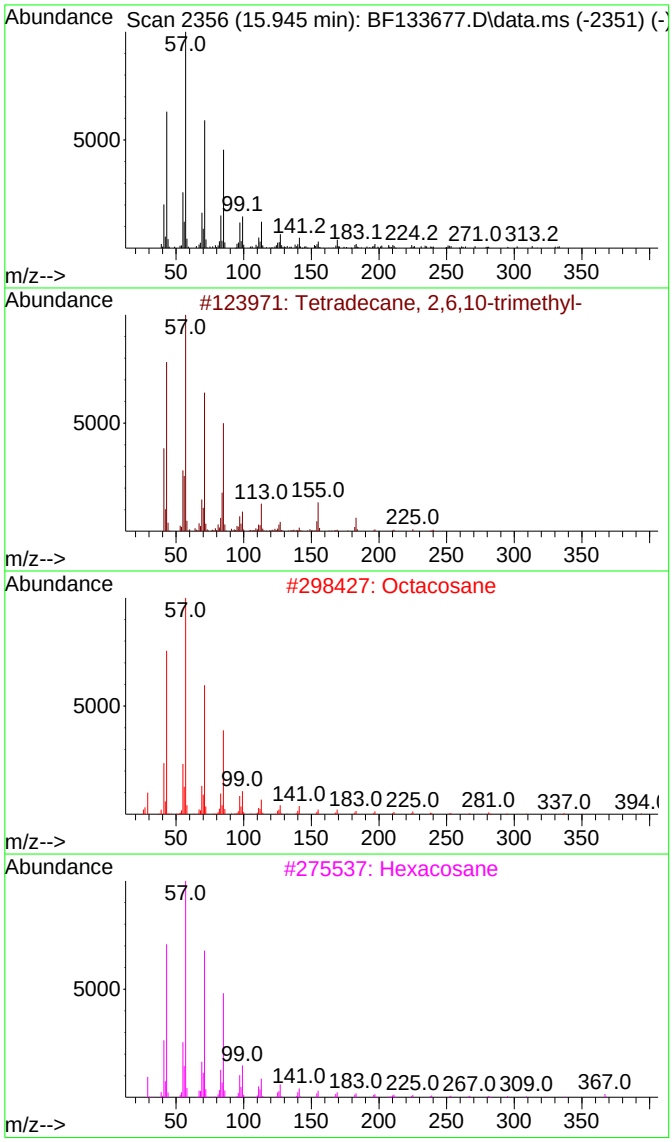
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

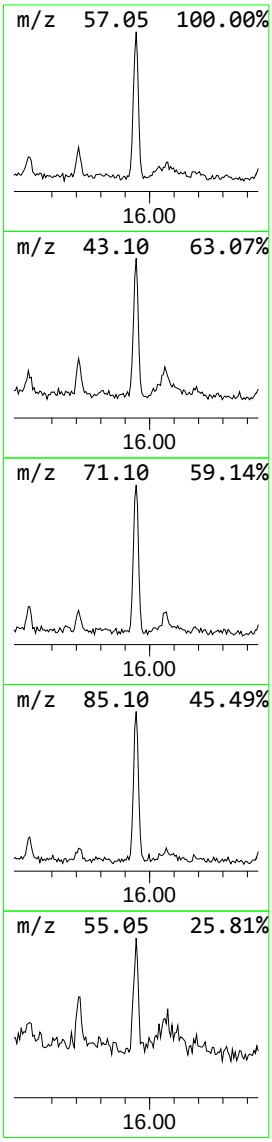
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 16 Tetradecane, 2,6,10-trimethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.945	6.82 ng	202975	Perylene-d12	15.474

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetradecane, 2,6,10-trimethyl-	240	C17H36	014905-56-7	93
2	Octacosane	394	C28H58	000630-02-4	90
3	Hexacosane	366	C26H54	000630-01-3	90
4	Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	87
5	Eicosane, 1-iodo-	408	C20H41I	1000406-31-8	87





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ClientSampleId :
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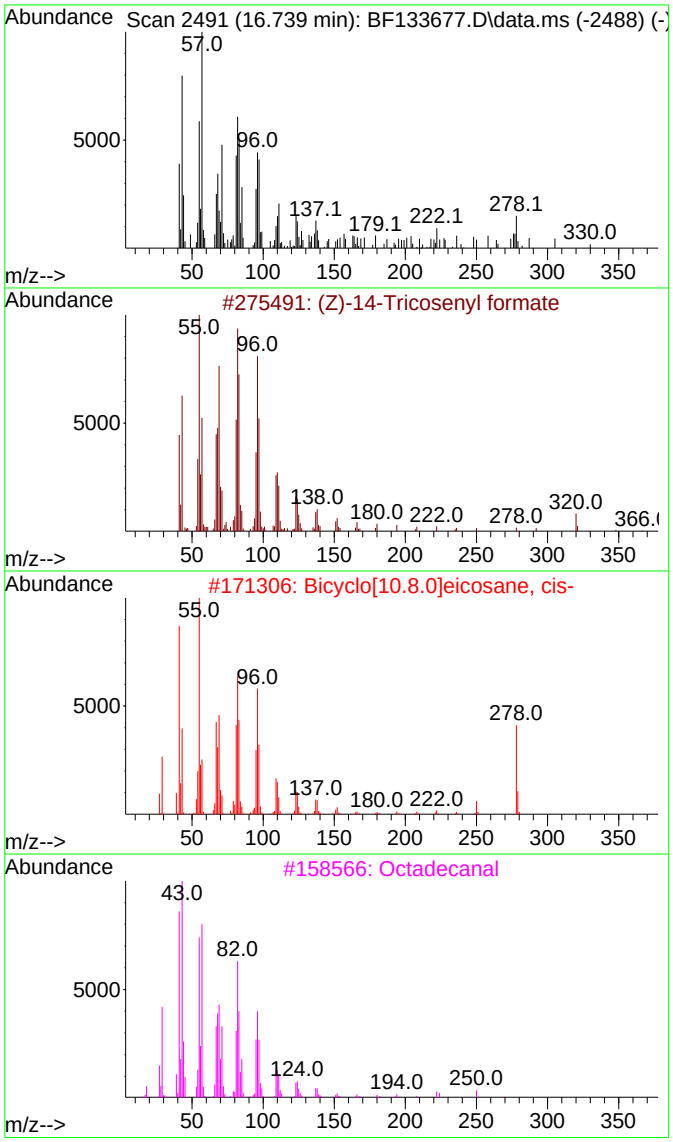
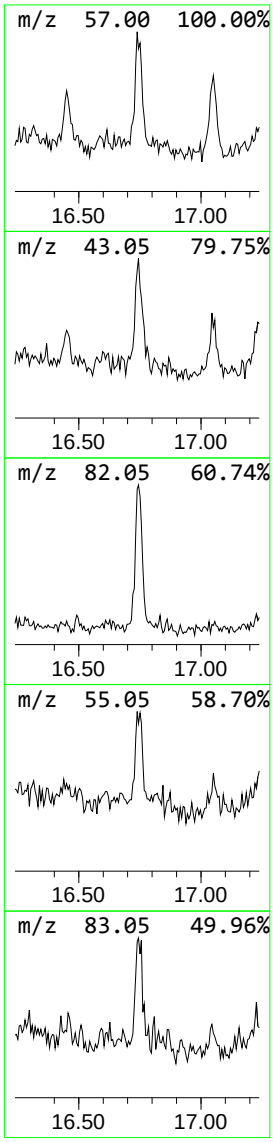
Peak Number 17 (Z)-14-Tricosenyl formate Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.739	4.26 ng	126800	Perylene-d12	15.474

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(Z)-14-Tricosenyl formate	366	C24H46O2	077899-10-6	62
2	Bicyclo[10.8.0]eicosane, cis-	278	C20H38	1000155-82-2	55
3	Octadecanal	268	C18H36O	000638-66-4	53
4	Oxirane, heptadecyl-	282	C19H38O	067860-04-2	49
5	Hexadecanal	240	C16H32O	000629-80-1	49





Tentatively Identified Compound (LSC) summary

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2-Pentanone, 4-...	5.051	2.0	ng	64947	1	6.833	647837	20.0
Decahydro-1,1,4...	9.274	2.4	ng	127626	3	9.880	1063680	20.0
1H-Indene, octa...	9.580	4.1	ng	220048	3	9.880	1063680	20.0
unknown9.627	9.627	4.8	ng	255420	3	9.880	1063680	20.0
unknown9.745	9.745	5.0	ng	264720	3	9.880	1063680	20.0
Cyclohexane, 1,...	9.786	6.6	ng	351994	3	9.880	1063680	20.0
unknown10.139	10.139	3.6	ng	189630	3	9.880	1063680	20.0
2,11-Dioxabicyc...	10.286	7.4	ng	394580	3	9.880	1063680	20.0
Pentadecane, 2,...	10.533	5.7	ng	300277	3	9.880	1063680	20.0
Pentadecane, 2,...	10.804	36.7	ng	1293600	4	11.374	705433	20.0
Heptadecane, 2,...	11.274	32.3	ng	1139690	4	11.374	705433	20.0
unknown14.521	14.521	6.0	ng	171954	5	14.015	574301	20.0
Benzo[e]pyrene	15.045	2.5	ng	74365	6	15.474	595511	20.0
Heneicosane	15.127	7.6	ng	225619	6	15.474	595511	20.0
Oxirane, hexade...	15.709	2.5	ng	73717	6	15.474	595511	20.0
Tetradecane, 2,...	15.945	6.8	ng	202975	6	15.474	595511	20.0
(Z)-14-Tricosen...	16.739	4.3	ng	126800	6	15.474	595511	20.0