LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082124\
Data File : BF139093.D
Acq On : 21 Aug 2024 10:51
Operator : RC/JU
Sample : P3663-04
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
914-J-SD-0-1-081624

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-BF082024.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF139093.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	14	25	38	rVB	1219453	2045592	79.31%	10.148%
2	3.428	219	227	240	rBV	43896	97393	3.78%	0.483%
3	4.010	319	326	332	rBV	23930	37219	1.44%	0.185%
4	5.122	507	515	521	rBV	95981	162454	6.30%	0.806%
5	5.516	575	582	587	rBV	1836993	2473196	95.89%	12.269%
6	6.516	745	752	757	rBV	1826129	2579329	100.00%	12.796%
7	6.716	781	786	792	rBV	27126	34452	1.34%	0.171%
8	6.893	811	816	821	rVB	441281	561800	21.78%	2.787%
9	7.051	833	843	848	rBV	141936	178344	6.91%	0.885%
10	7.457	905	912	917	rBV	1150782	1565986	60.71%	7.769%
11	8.175	1029	1034	1039	rBV	579557	726842	28.18%	3.606%
12	8.487	1082	1087	1095	rBV	46166	59768	2.32%	0.296%
13	9.251	1211	1217	1222	rBV	1953716	2466234	95.62%	12.235%
14	9.928	1327	1332	1337	rBV	656077	840081	32.57%	4.167%
15	10.028	1343	1349	1356	rBV2	49664	82756	3.21%	0.411%
16	10.716	1459	1466	1471	rBV	1354141	1719434	66.66%	8.530%
17	11.416	1574	1585	1590	rBV	685813	854010	33.11%	4.237%
18	11.533	1600	1605	1609	rBV3	50434	75305	2.92%	0.374%
19	11.851	1655	1659	1665	rVB2	77736	103071	4.00%	0.511%
20	11.945	1668	1675	1683	rBV2	123241	214149	8.30%	1.062%
21	12.727	1804	1808	1817	rBV	48691	74619	2.89%	0.370%
22	12.951	1842	1846	1850	rBV	36218	44690	1.73%	0.222%
23	13.004	1850	1855	1860	rVB	1449181	1795746	69.62%	8.908%
24	13.904	2003	2008	2017	rBV	103396	164019	6.36%	0.814%
25	14.051	2028	2033	2039	rBV	334637	424788	16.47%	2.107%
26	14.545	2112	2117	2123	rBV	66315	112469	4.36%	0.558%
27	15.198	2223	2228	2230	rBV	22867	32912	1.28%	0.163%
28	15.527	2279	2284	2291	rBV	310779	469959	18.22%	2.331%
29	16.086	2375	2379	2388	rVV2	17898	35609	1.38%	0.177%
30	17.727	2652	2658	2671	rVB8	19697	53378	2.07%	0.265%
31	17.980	2694	2701	2710	rBV5	15309	36410	1.41%	0.181%
32	18.221	2735	2742	2751	rVB8	13170	35990	1.40%	0.179%

Sum of corrected areas: 20158004

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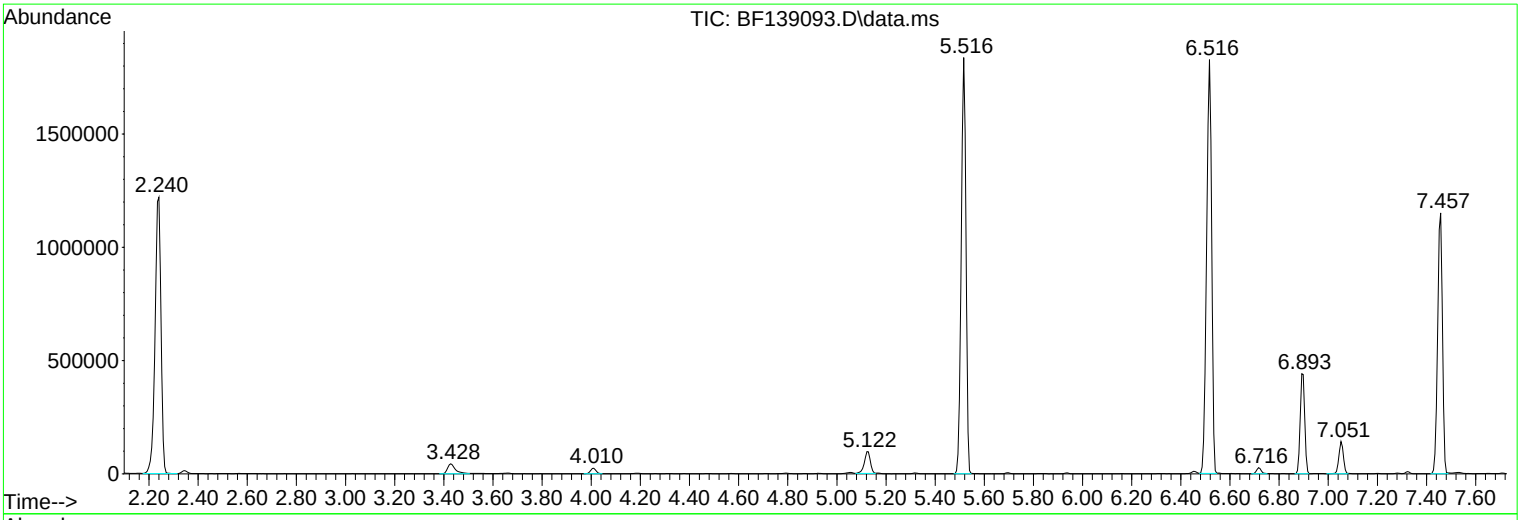
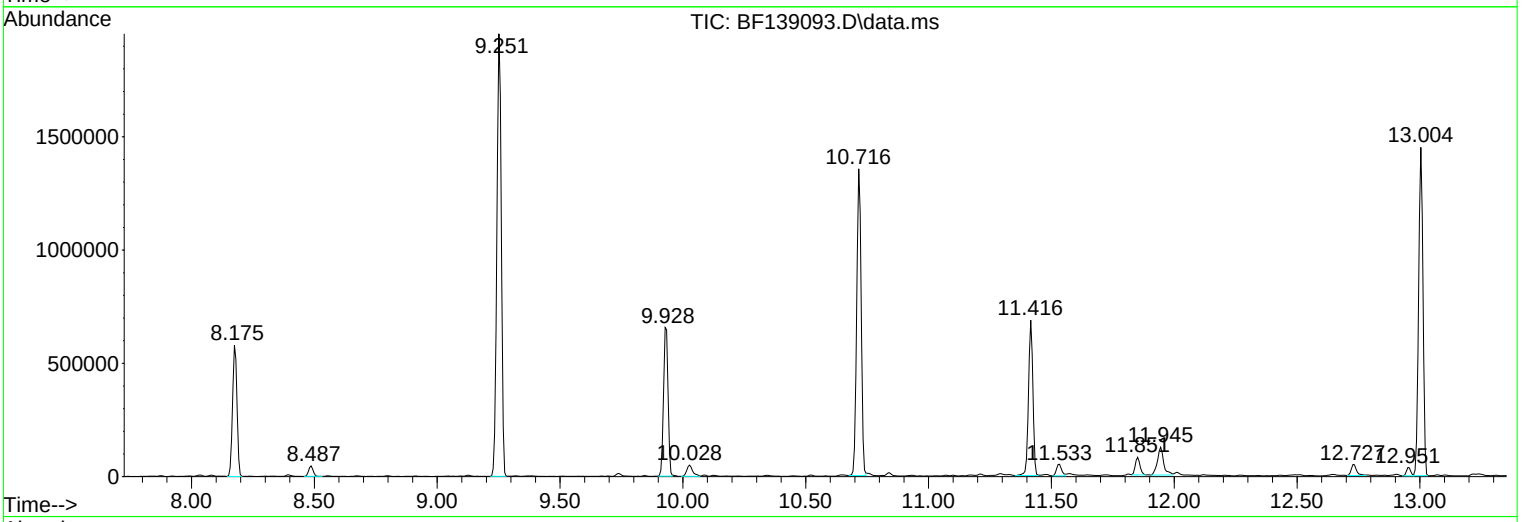
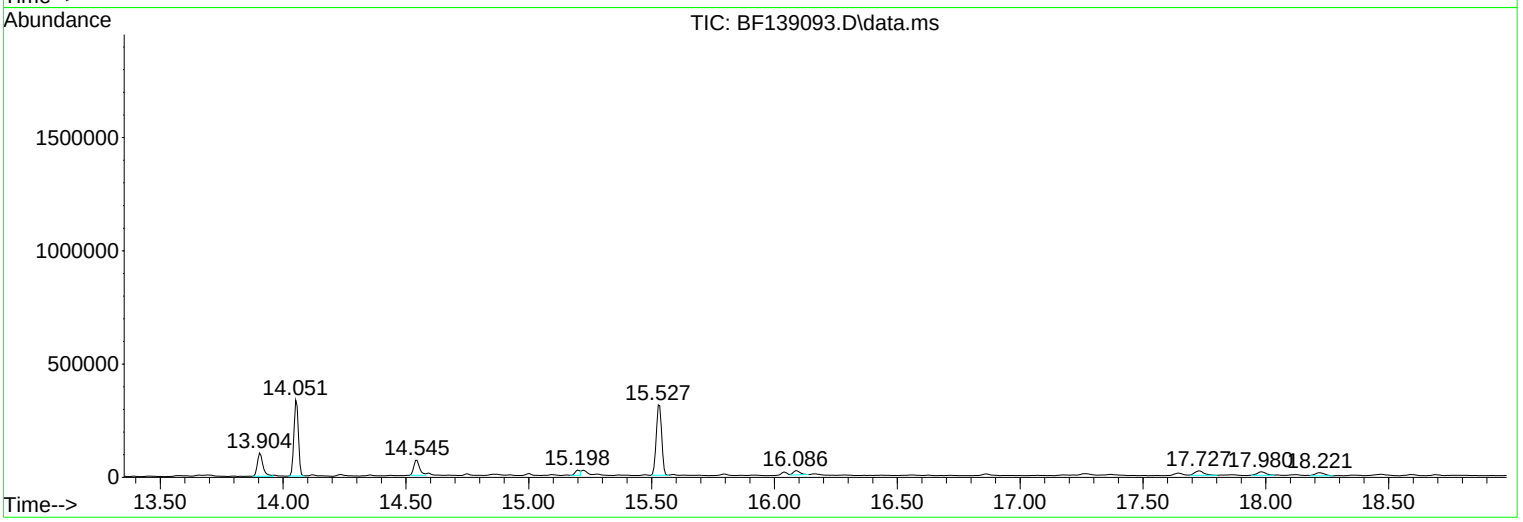
914-J-SD-0-1-081624

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF082024.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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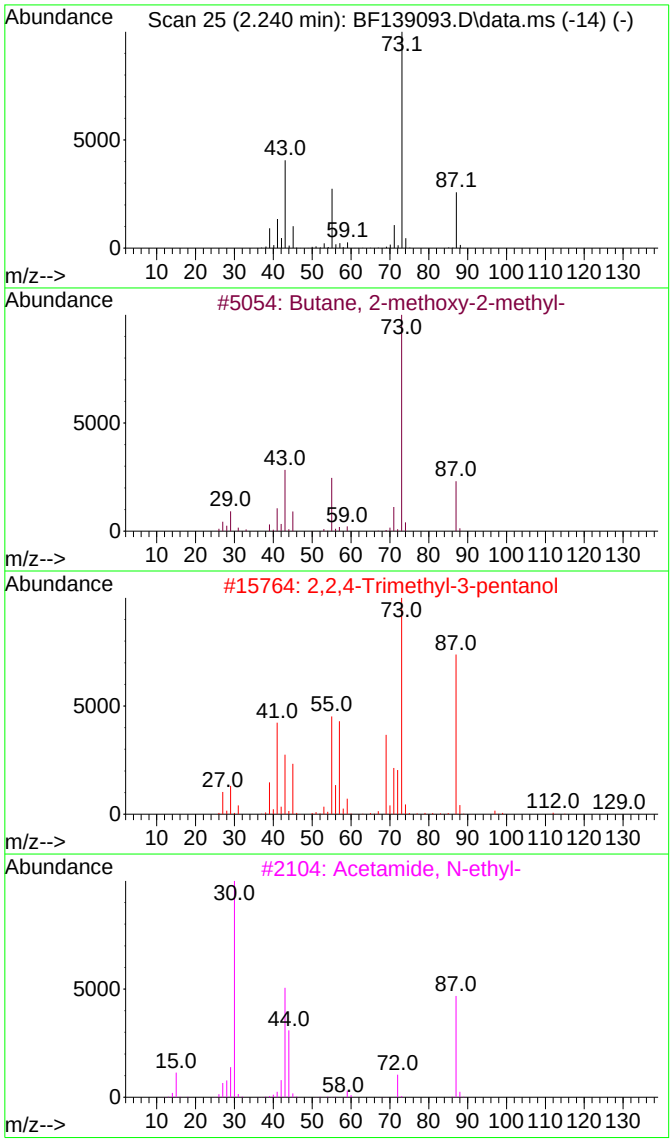
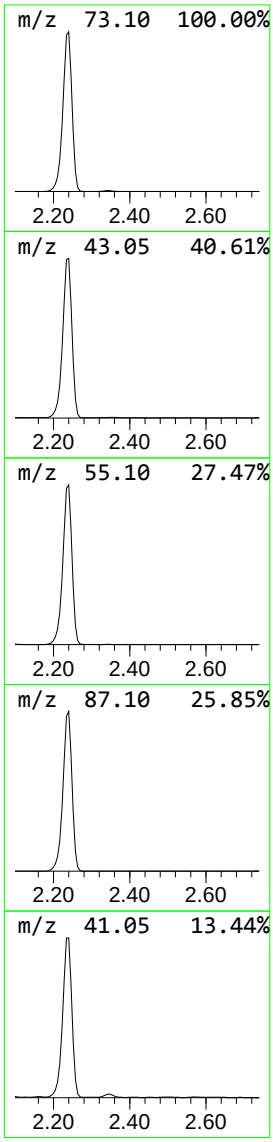
****

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.240	72.82 ng	2045590	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	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	27
4	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
5	Octanal, 7-methoxy-3,7-dimethyl-	186	C11H22O2	003613-30-7	17





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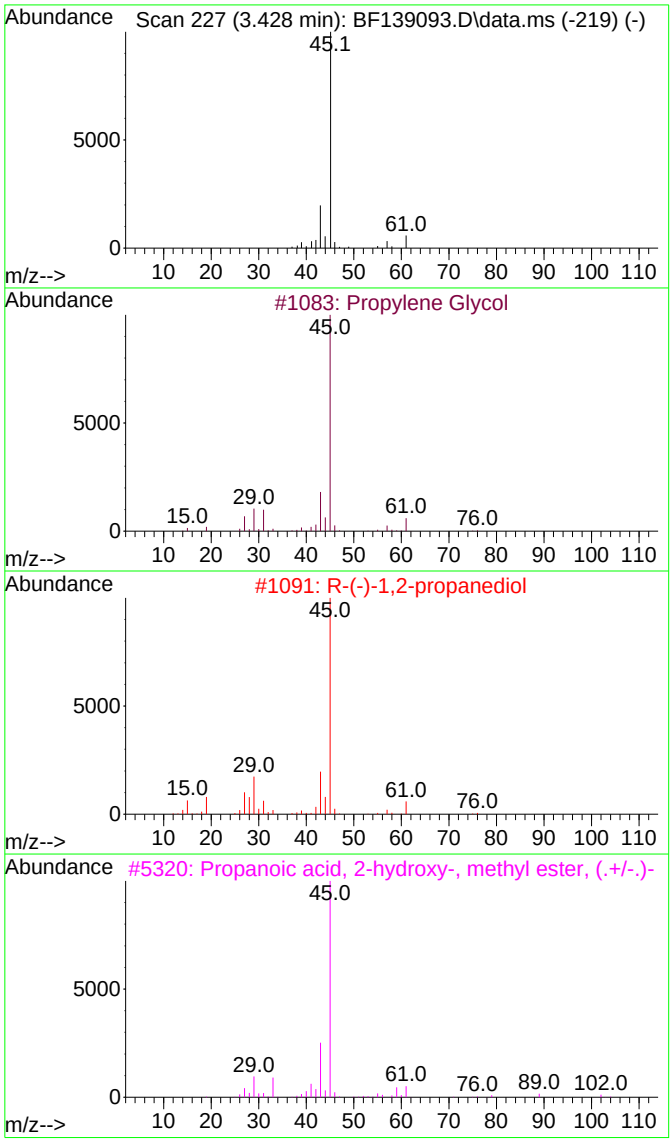
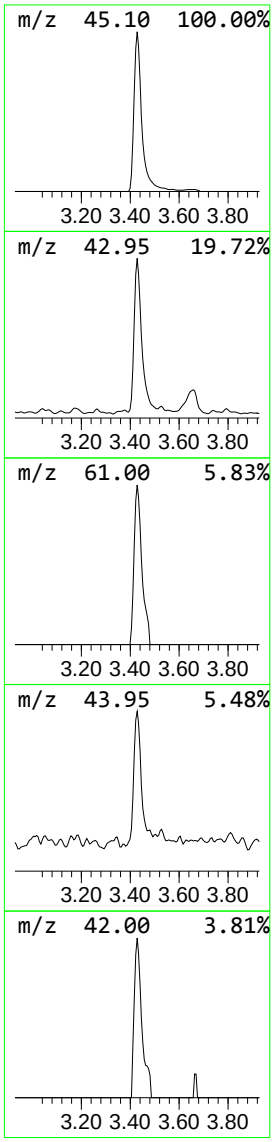
****

Peak Number 2 unknown3.428 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.428	3.47 ng	97393	1,4-Dichlorobenzene-d4	6.898

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propylene Glycol	76	C3H8O2	000057-55-6	43
2	R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	43
3	Propanoic acid, 2-hydroxy-, meth...	104	C4H8O3	000547-64-8	9
4	Isopropyl Alcohol	60	C3H8O	000067-63-0	9
5	Formamide	45	CH3NO	000075-12-7	5





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ALS Vial : 6 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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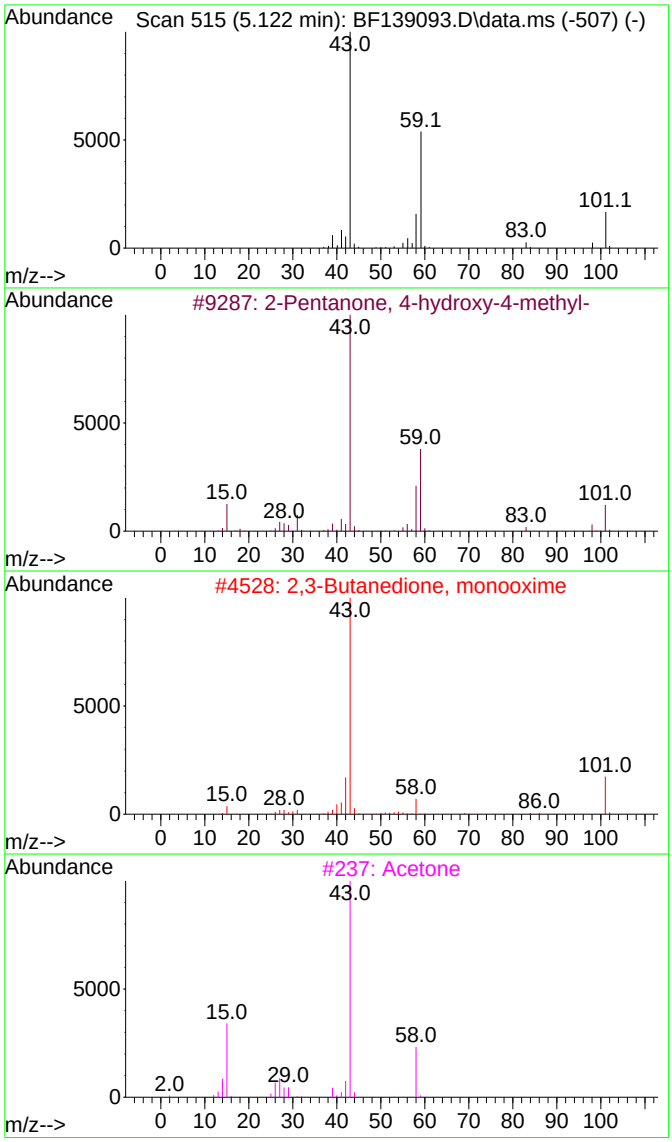
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF082024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

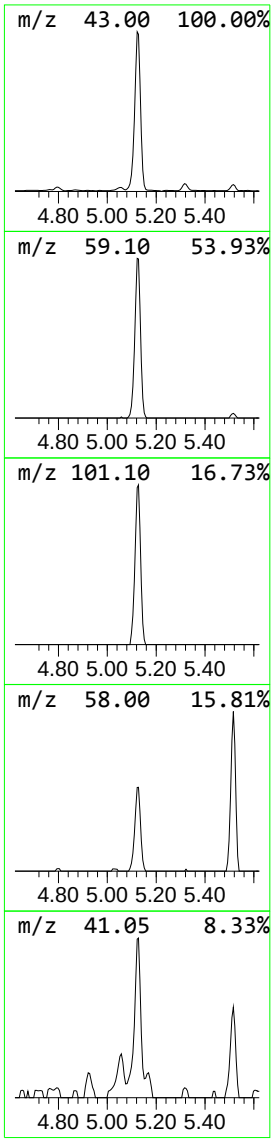
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.122	5.78 ng	162454	1,4-Dichlorobenzene-d4	6.898

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16
3	Acetone	58	C3H6O	000067-64-1	12
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12
5	2-Propanone, 1-(1-methylethoxy)-	116	C6H12O2	042781-12-4	9





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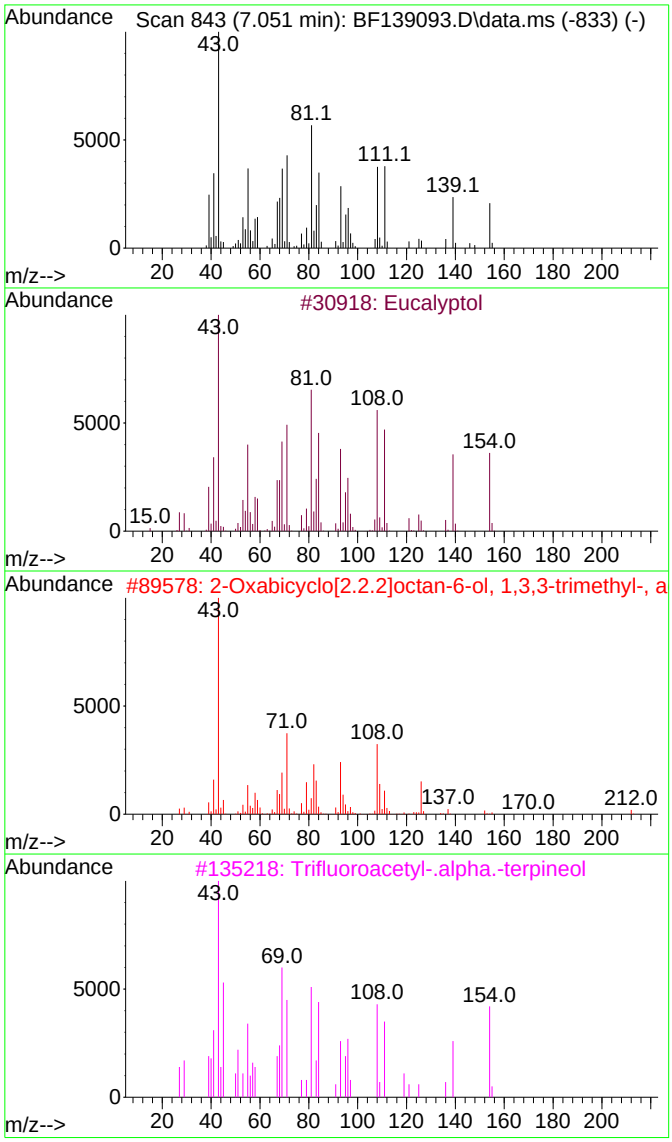
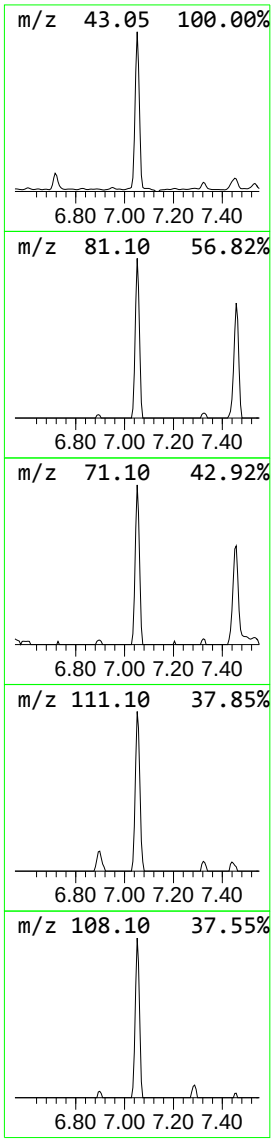
****

Peak Number 4 Eucalyptol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.051	6.35 ng	178344	1,4-Dichlorobenzene-d4	6.898

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eucalyptol	154	C10H18O	000470-82-6	97
2	2-Oxabicyclo[2.2.2]octan-6-ol, 1...	212	C12H20O3	057709-95-2	47
3	Trifluoroacetyl-.alpha.-terpineol	250	C12H17F3O2	1000058-17-6	42
4	2-Acetylcyclopentanone	126	C7H10O2	001670-46-8	27
5	2-Isopropyl-5-methylhex-2-enal	154	C10H18O	035158-25-9	25





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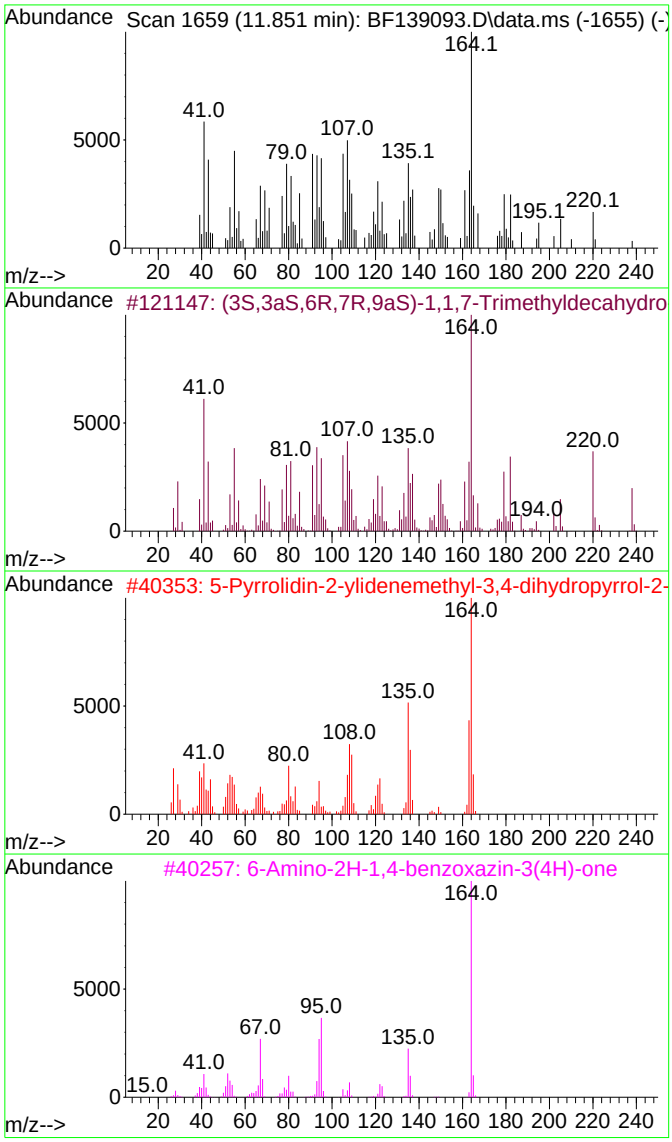
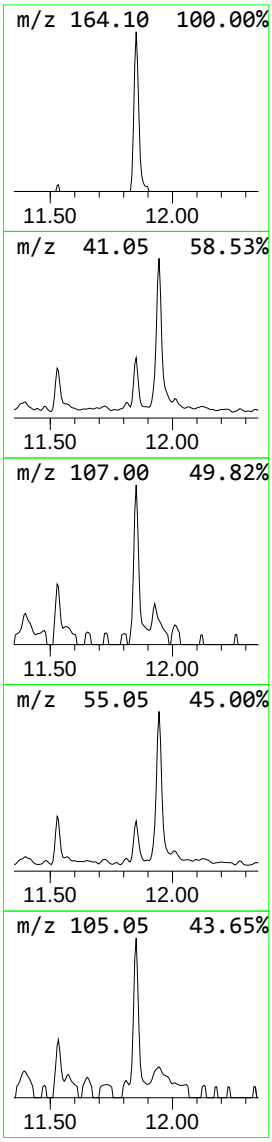
****
Peak Number 5 (3S,3aS,6R,7R,9aS)-1,1,7-Tr... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.851	2.41 ng	103071	Phenanthrene-d10	11.416

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(3S,3aS,6R,7R,9aS)-1,1,7-Trimeth...	238	C15H26O2	002649-64-1	99
2	5-Pyrrolidin-2-ylidenemethyl-3,4...	164	C9H12N2O	1010192-09-5	46
3	6-Amino-2H-1,4-benzoxazin-3(4H)-one	164	C8H8N2O2	089976-75-0	35
4	1(3H)-Isobenzofuranone, 6-hydraz...	164	C8H8N2O2	1000362-60-8	30
5	N-(3,4-Dimethoxyphenethyl)-2-(4-...	383	C24H33NO3	1000498-03-0	27





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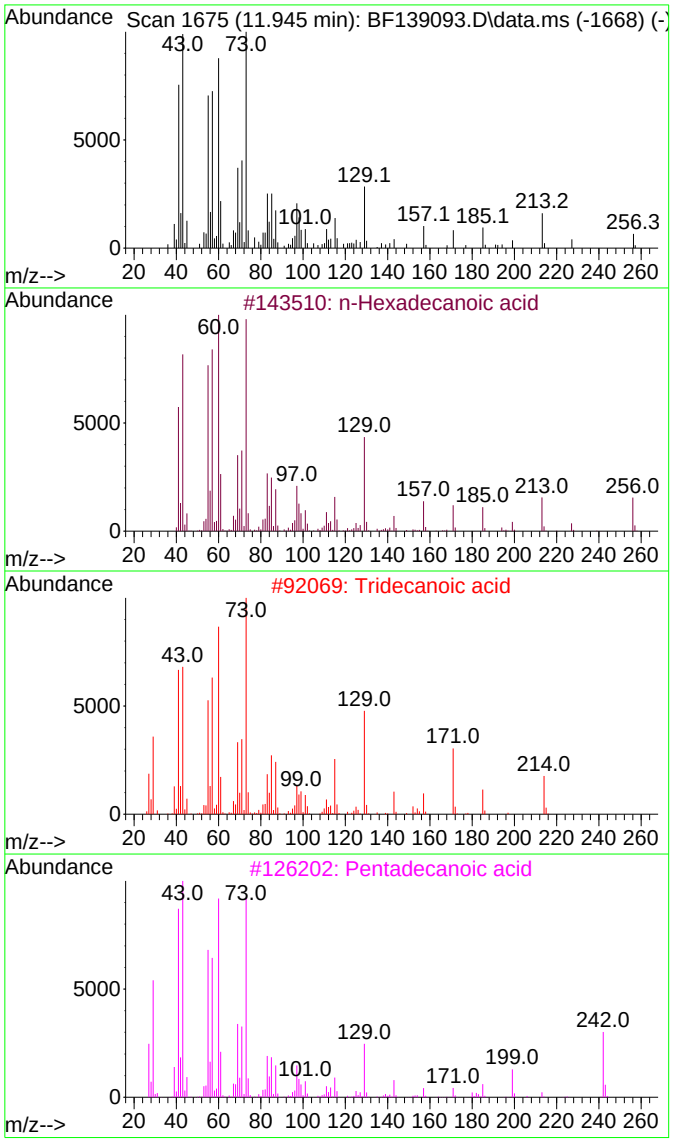
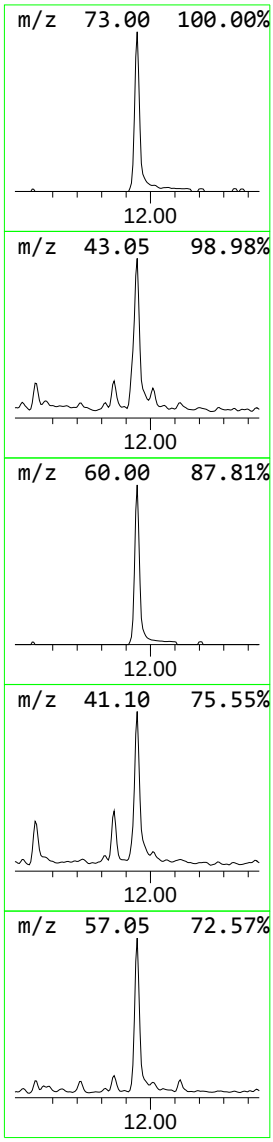
****

Peak Number 6 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.945	5.02 ng	214149	Phenanthrene-d10	11.416

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tridecanoic acid	214	C13H26O2	000638-53-9	92
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
4	Oxalic acid, allyl pentadecyl ester	340	C20H36O4	1000309-24-3	20
5	Oxalic acid, allyl hexadecyl ester	354	C21H38O4	1000309-24-4	20





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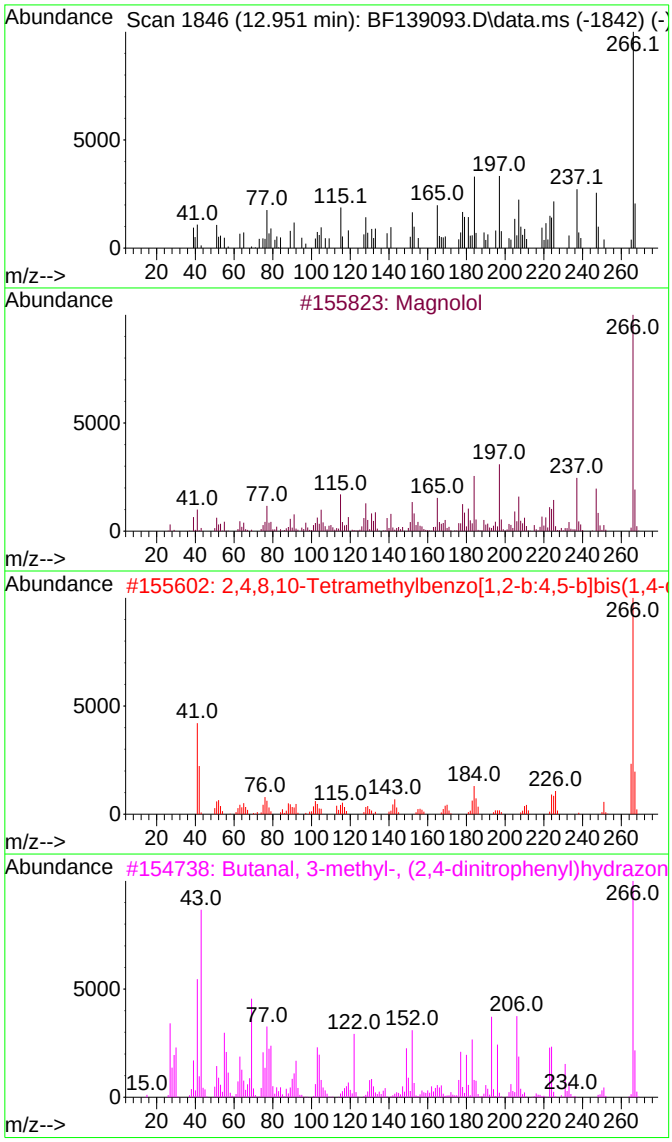
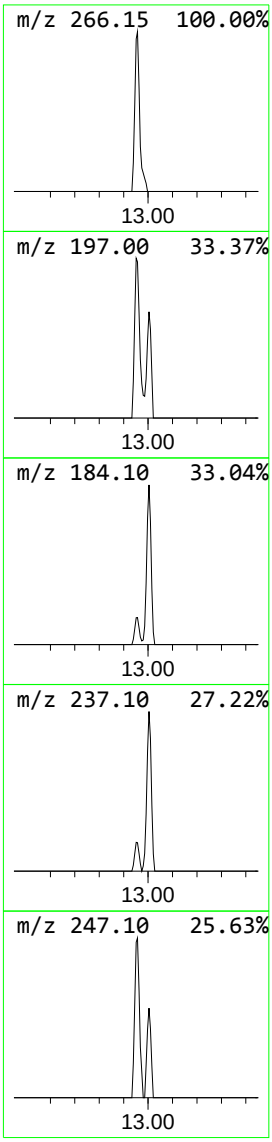
****

Peak Number 7 Magnolol Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.951	2.10 ng	44690	Chrysene-d12	14.051

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Magnolol	266	C18H18O2	000528-43-8	99
2	2,4,8,10-Tetramethylbenzo[1,2-b:...	266	C16H18N4	017377-04-7	46
3	Butanal, 3-methyl-, (2,4-dinitro...	266	C11H14N4O4	002256-01-1	46
4	Perylene, 1,2,3,3a,4,5,6,7,8,9,9...	266	C20H26	007594-86-7	43
5	4-(5-Phenyl-2-pyrazolin-3-yl)tro...	266	C16H14N2O2	001033-52-9	43





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TIC Library : C:\Database\NIST20.L
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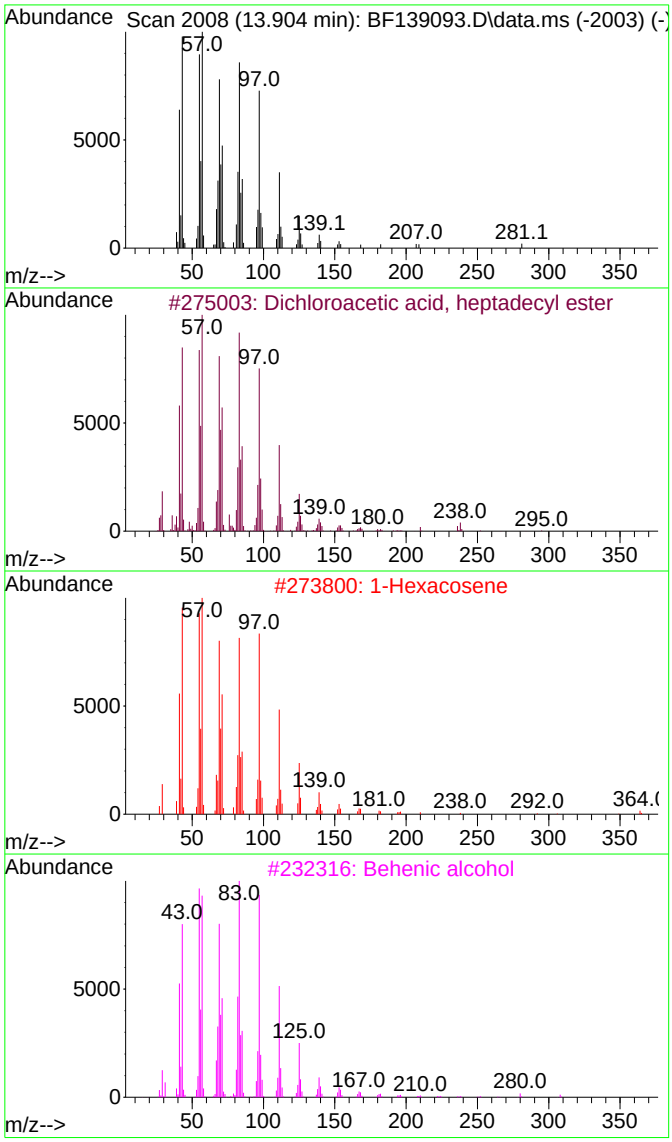
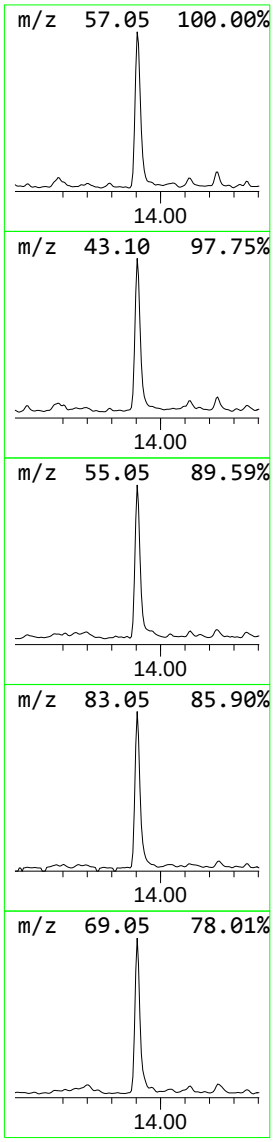
****
Peak Number 8 Dichloroacetic acid, heptad... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.904	7.72 ng	164019	Chrysene-d12	14.051

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	95
2	1-Hexacosene	364	C26H52	018835-33-1	94
3	Behenic alcohol	326	C22H46O	000661-19-8	94
4	Carbonic acid, octadecyl 2,2,2-t...	444	C21H39Cl3O3	1000314-56-3	94
5	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	94





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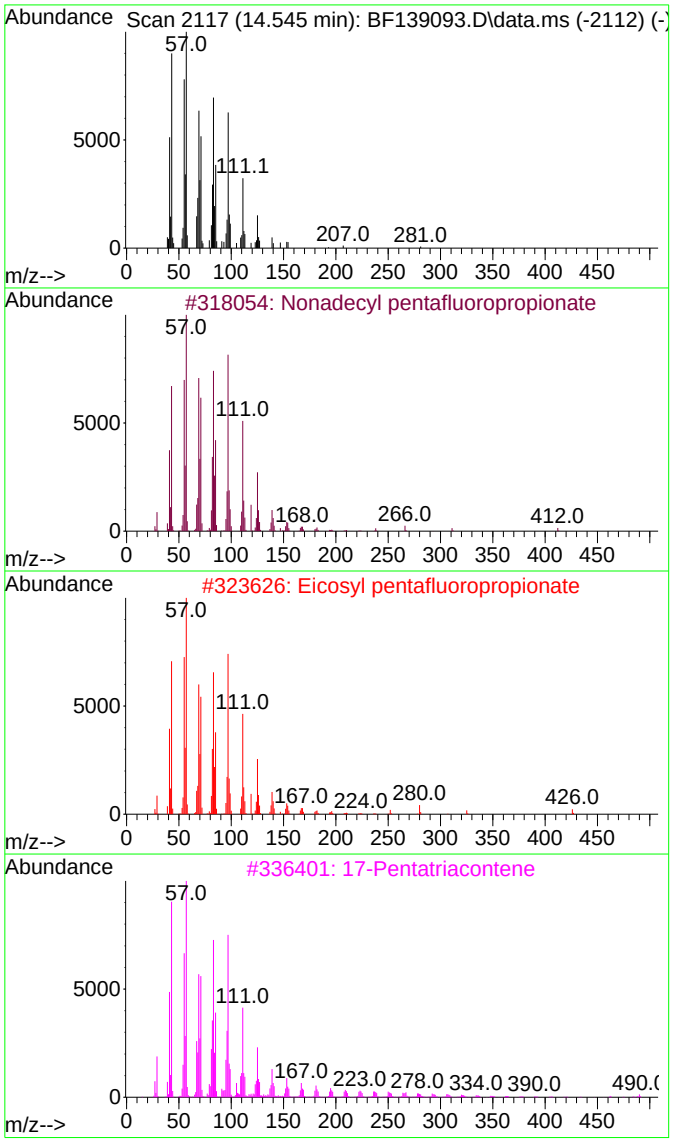
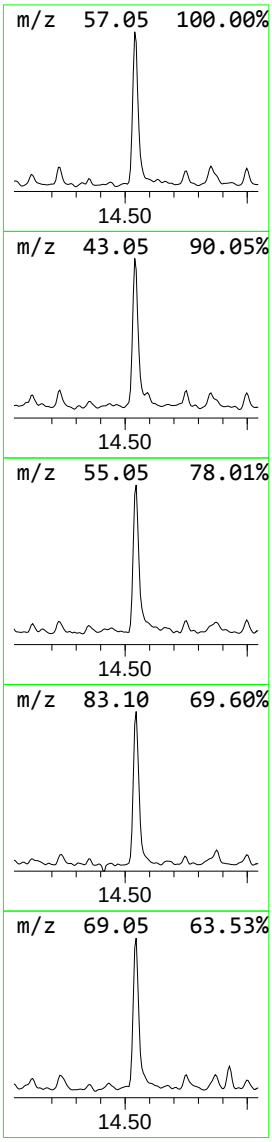
****
Peak Number 9 Nonadecyl pentafluoropropio... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.545	5.30 ng	112469	Chrysene-d12	14.051

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonadecyl pentafluoropropionate	430	C22H39F5O2	1000351-88-8	91
2	Eicosyl pentafluoropropionate	444	C23H41F5O2	1000351-80-8	91
3	17-Pentatriacontene	491	C35H70	006971-40-0	91
4	Hexadecyl propyl ether	284	C19H40O	1000406-27-9	91
5	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	91





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082124\
Data File : BF139093.D
Acq On : 21 Aug 2024 10:51
Operator : RC/JU
Sample : P3663-04
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
914-J-SD-0-1-081624

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF082024.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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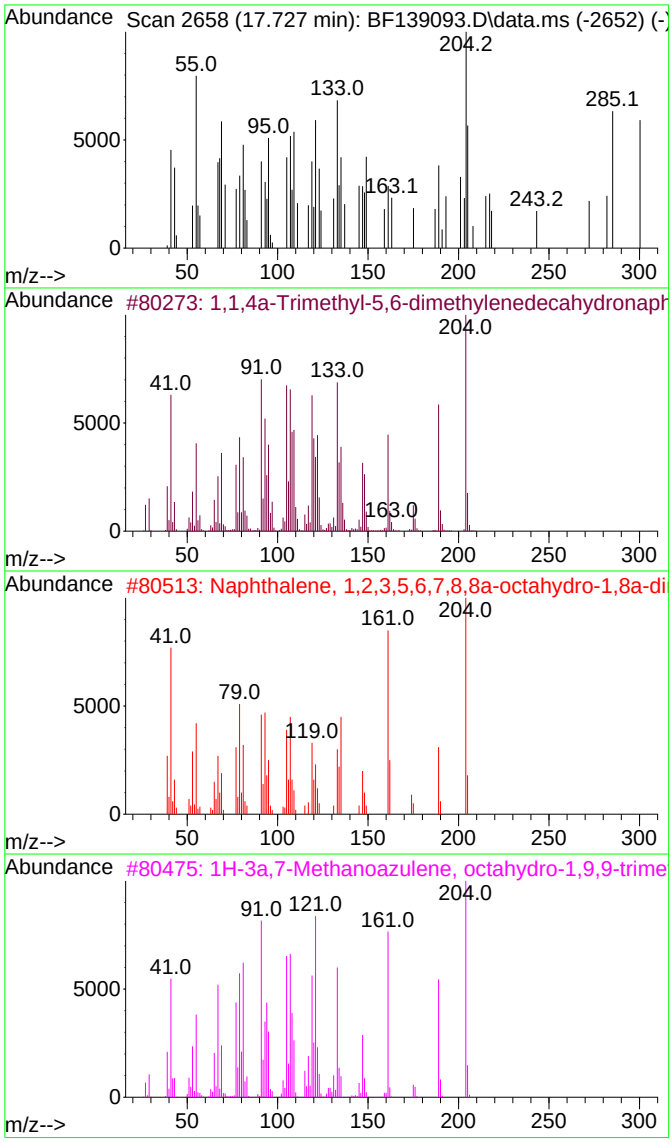
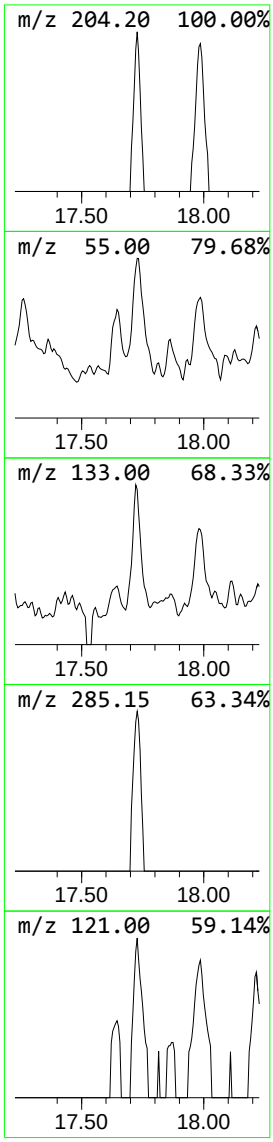
Peak Number 10 unknown17.727 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.727	2.27 ng	53378	Perylene-d12	15.533

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,1,4a-Trimethyl-5,6-dimethylene...	204	C15H24	1000193-60-8	38
2	Naphthalene, 1,2,3,5,6,7,8,8a-oc...	204	C15H24	004630-07-3	38
3	1H-3a,7-Methanoazulene, octahydr...	204	C15H24	000508-55-4	30
4	Humulane-1,6-dien-3-ol	222	C15H26O	1000140-23-1	27
5	Himachala-2,4-diene	204	C15H24	060909-27-5	25





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082124\
Data File : BF139093.D
Acq On : 21 Aug 2024 10:51
Operator : RC/JU
Sample : P3663-04
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
914-J-SD-0-1-081624

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF082024.M
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
Butane, 2-metho...	2.240	72.8	ng	2045590	1	6.898	561800	20.0
unknown3.428	3.428	3.5	ng	97393	1	6.898	561800	20.0
2-Pentanone, 4-...	5.122	5.8	ng	162454	1	6.898	561800	20.0
Eucalyptol	7.051	6.3	ng	178344	1	6.898	561800	20.0
(3S,3aS,6R,7R,9...	11.851	2.4	ng	103071	4	11.416	854010	20.0
n-Hexadecanoic ...	11.945	5.0	ng	214149	4	11.416	854010	20.0
Magnolol	12.951	2.1	ng	44690	5	14.051	424788	20.0
Dichloroacetic ...	13.904	7.7	ng	164019	5	14.051	424788	20.0
Nonadecyl penta...	14.545	5.3	ng	112469	5	14.051	424788	20.0
unknown17.727	17.727	2.3	ng	53378	6	15.533	469959	20.0