LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF022122\
Data File : BF126995.D
Acq On : 22 Feb 2022 01:28
Operator : CG\JU
Sample : N1602-08
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
20220084A-AMEDNDED-BERKELEY-8A-COMP

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-BF021622.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF126995.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.163	485	489	497	rBV	96550	124746	3.11%	0.532%
2	5.545	548	554	557	rBV	3016954	3190398	79.61%	13.598%
3	6.539	717	723	726	rBV	2838410	3535081	88.21%	15.067%
4	6.916	783	787	790	rBV	752442	570237	14.23%	2.430%
5	7.481	877	883	886	rBV	2376086	2341176	58.42%	9.978%
6	7.633	906	909	915	rVB2	62091	71438	1.78%	0.304%
7	8.092	983	987	997	rBV	201233	199099	4.97%	0.849%
8	8.198	1000	1005	1008	rBV	901606	766627	19.13%	3.267%
9	9.275	1182	1188	1191	rBV	4601820	4007480	100.00%	17.080%
10	9.351	1194	1201	1203	rBV2	40682	44402	1.11%	0.189%
11	9.957	1300	1304	1307	rVB	976090	849384	21.19%	3.620%
12	10.745	1434	1438	1441	rBV	2422978	2023404	50.49%	8.624%
13	10.874	1457	1460	1465	rVB	115999	110636	2.76%	0.472%
14	11.316	1533	1535	1542	rVB	68433	71729	1.79%	0.306%
15	11.445	1553	1557	1560	rBV	1090118	873133	21.79%	3.721%
16	11.827	1618	1622	1625	rVB	77977	65806	1.64%	0.280%
17	13.033	1822	1827	1830	rBV	3942467	3519074	87.81%	14.999%
18	13.457	1895	1899	1902	rBV	65282	58647	1.46%	0.250%
19	13.939	1975	1981	1992	rBV6	40222	141400	3.53%	0.603%
20	14.086	2002	2006	2009	rBV	486922	424235	10.59%	1.808%
21	15.580	2255	2260	2268	rBV	364904	474490	11.84%	2.022%

Sum of corrected areas: 23462622

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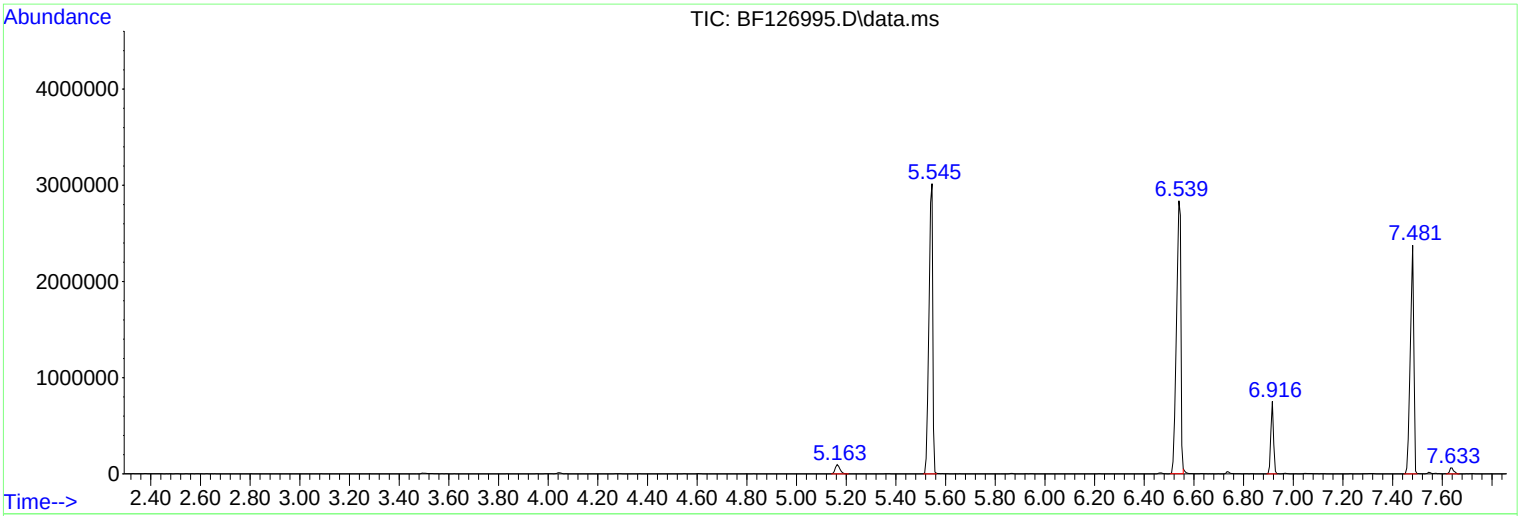
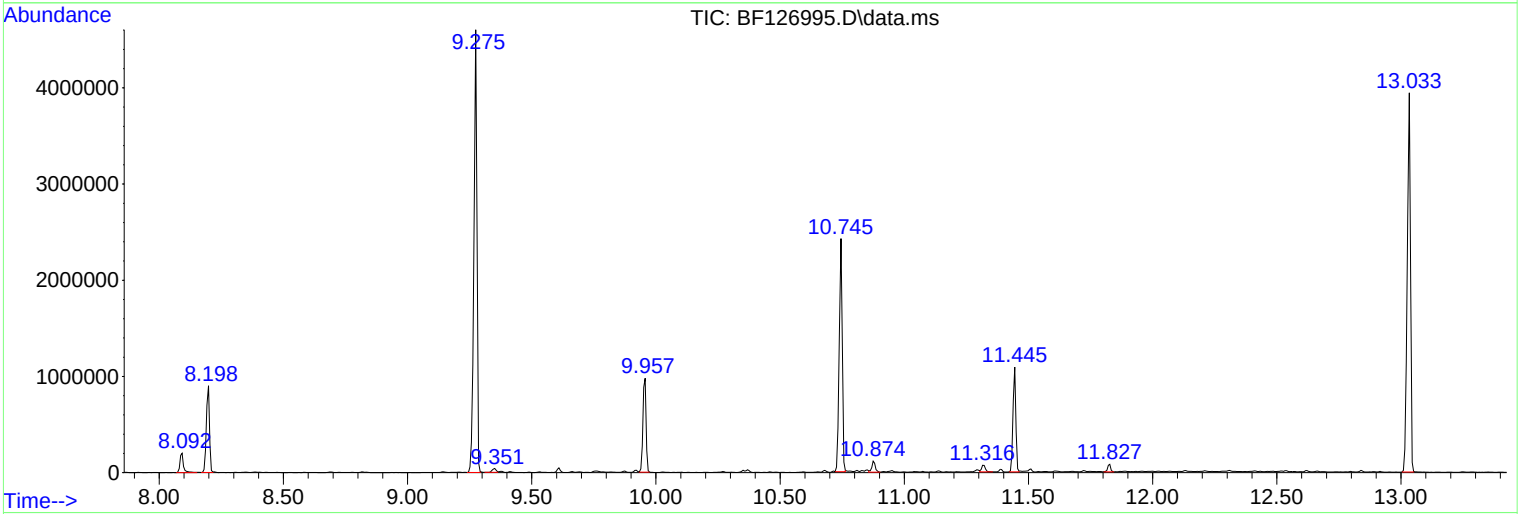
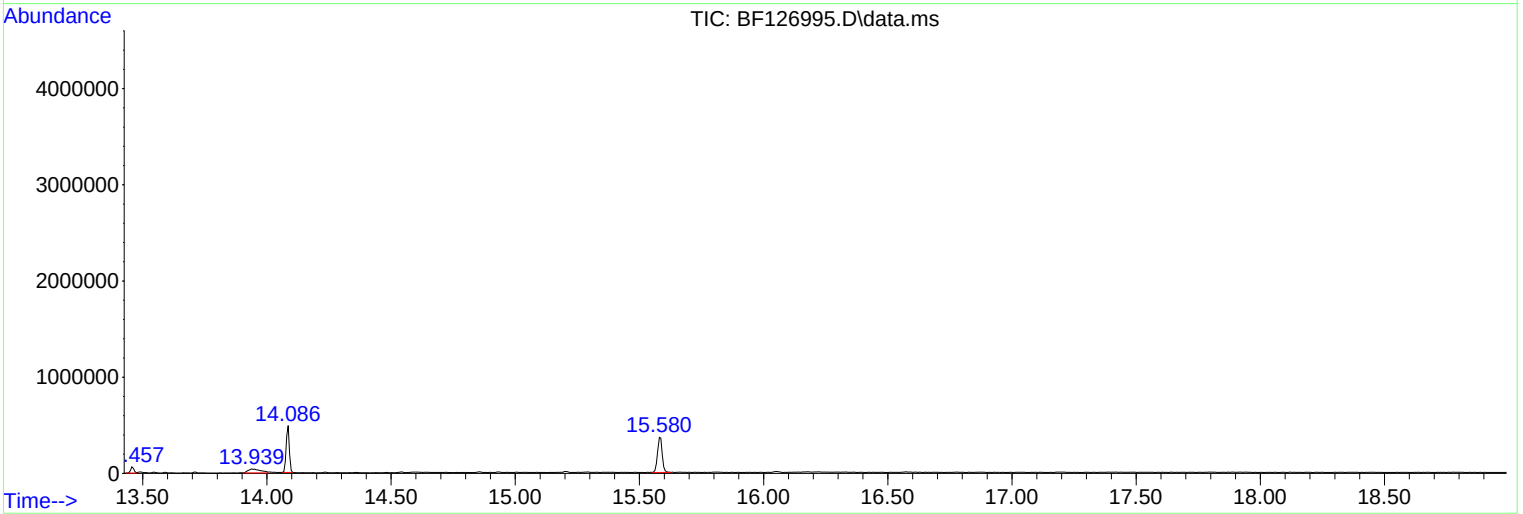
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF021622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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







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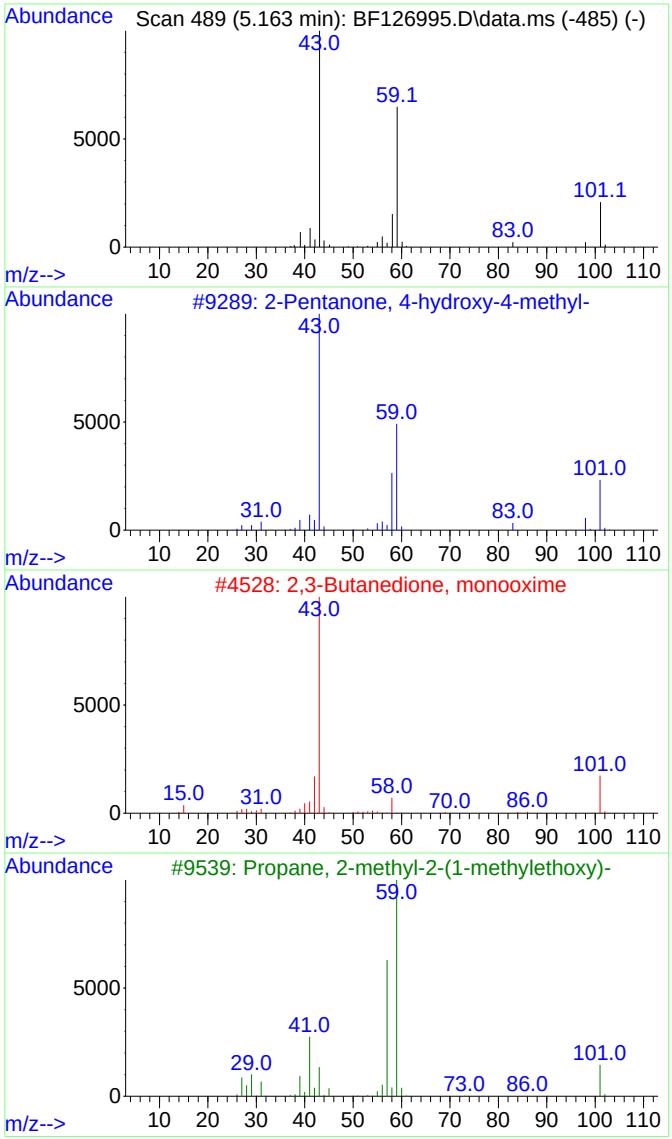
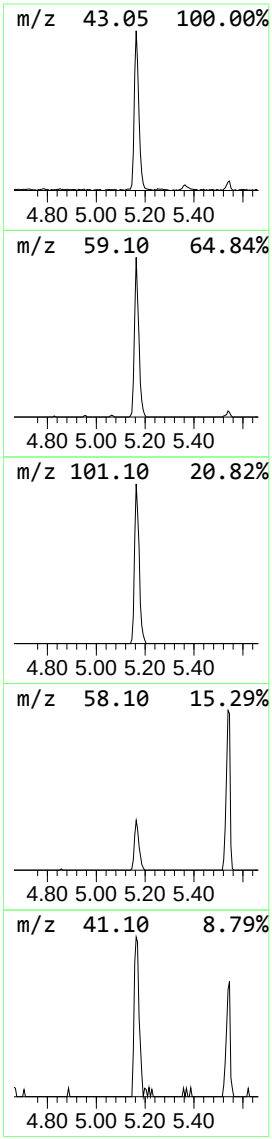
****
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.163	4.38 ng	124746	1,4-Dichlorobenzene-d4	6.916

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	35
3	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	33
4	3-Hexanol	102	C6H14O	000623-37-0	28
5	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	28





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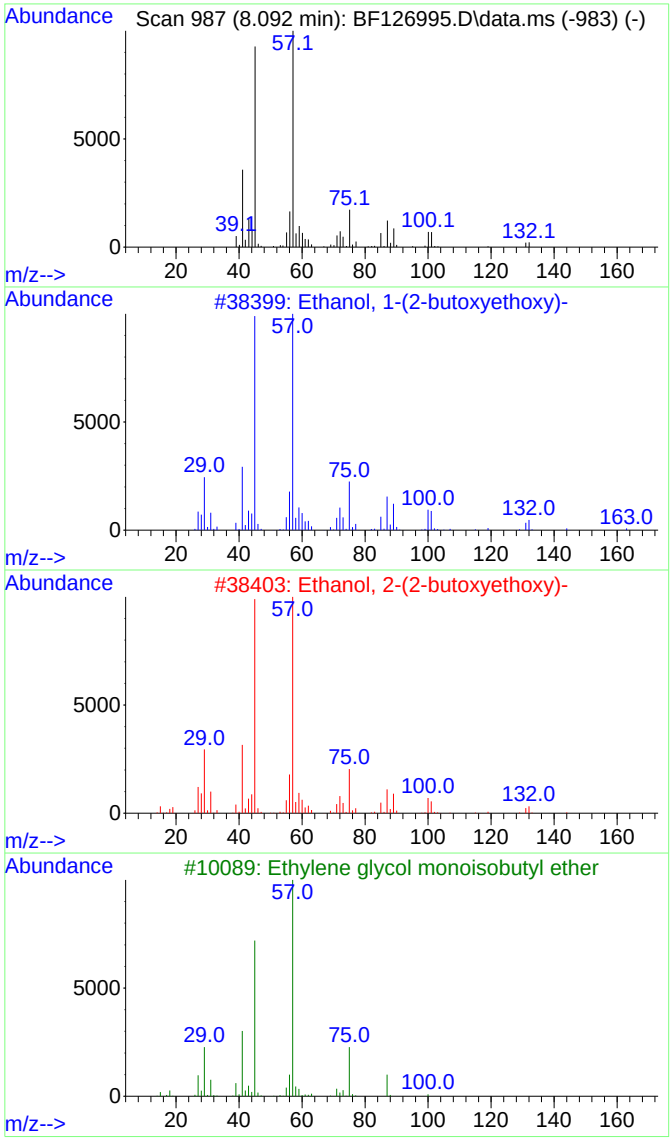
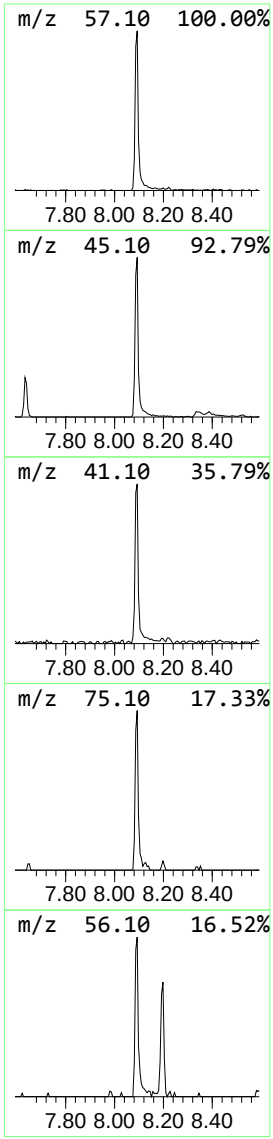
****
Peak Number 2 Ethanol, 1-(2-butoxyethoxy)- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.092	5.19 ng	199099	Naphthalene-d8	8.198

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	90
2	Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
3	Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	59
4	Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	56
5	Butane, 1-(1-methylpropoxy)-	130	C8H18O	000999-65-5	53





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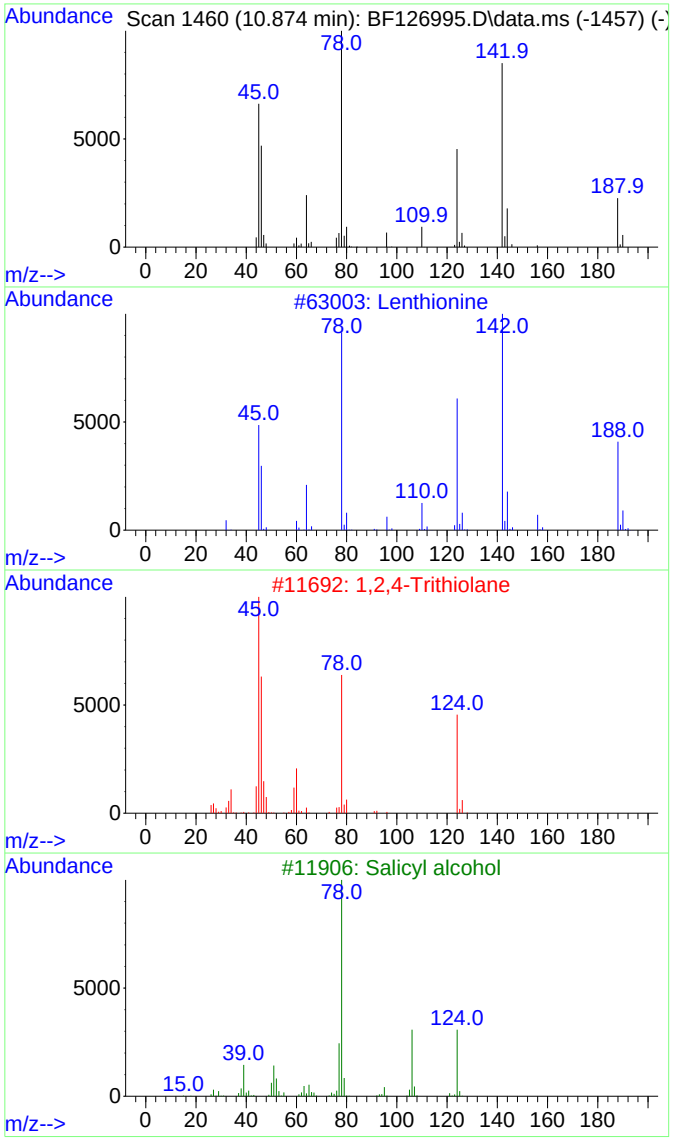
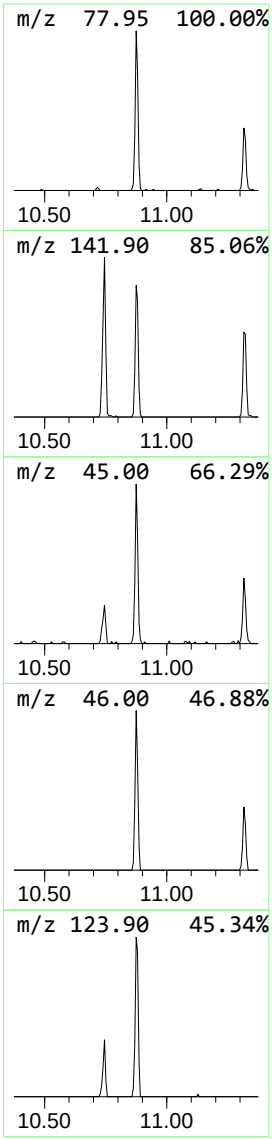
****

Peak Number 3 Lenthionine Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.874	2.53 ng	110636	Phenanthrene-d10	11.445

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Lenthionine	188	C2H4S5	000292-46-6	95
2	1,2,4-Trithiolane	124	C2H4S3	000289-16-7	59
3	Salicyl alcohol	124	C7H8O2	000090-01-7	47
4	1,2,4,6-Tetrathiepane	170	C3H6S4	000292-45-5	45
5	Phenylphosphonous acid	142	C6H7O2P	001779-48-2	40





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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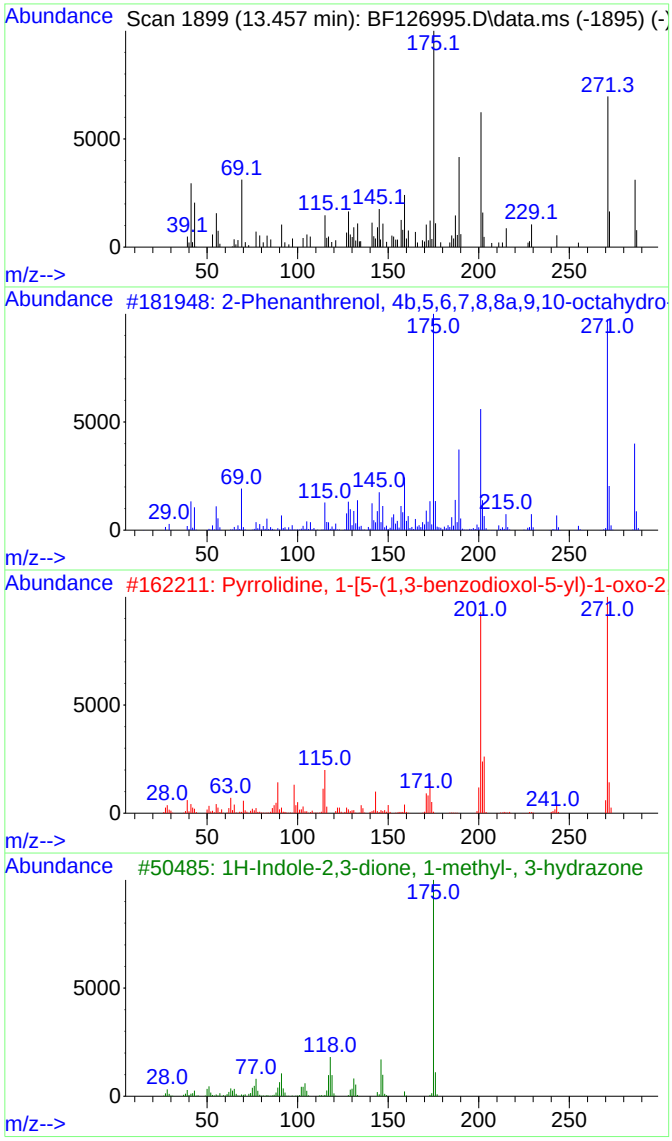
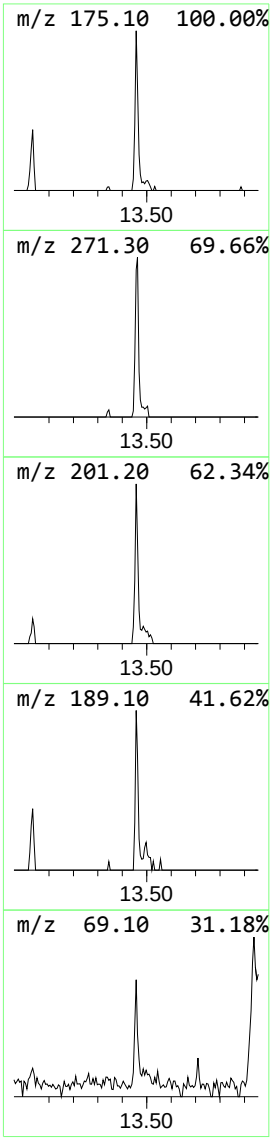
****
Peak Number 4 2-Phenanthrenol, 4b,5,6,7,8... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.457	2.76 ng	58647	Chrysene-d12	14.086

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Phenanthrenol, 4b,5,6,7,8,8a,9...	286	C20H30O	000511-15-9	95
2	Pyrrolidine, 1-[5-(1,3-benzodiox...	271	C16H17NO3	025924-78-1	30
3	1H-Indole-2,3-dione, 1-methyl-, ...	175	C9H9N3O	003265-23-4	18
4	2-Propenal, 3-[4-(dimethylamino)...	175	C11H13NO	006203-18-5	14
5	4-quinolinethiol, 2-methyl-	175	C10H9NS	1000404-71-3	14





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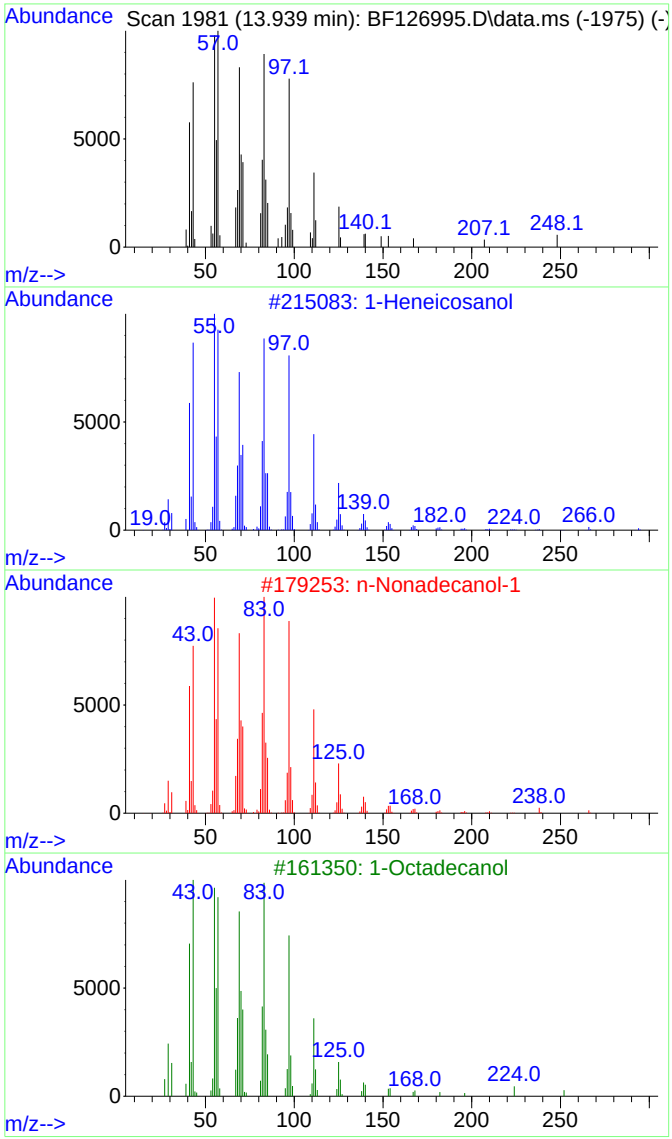
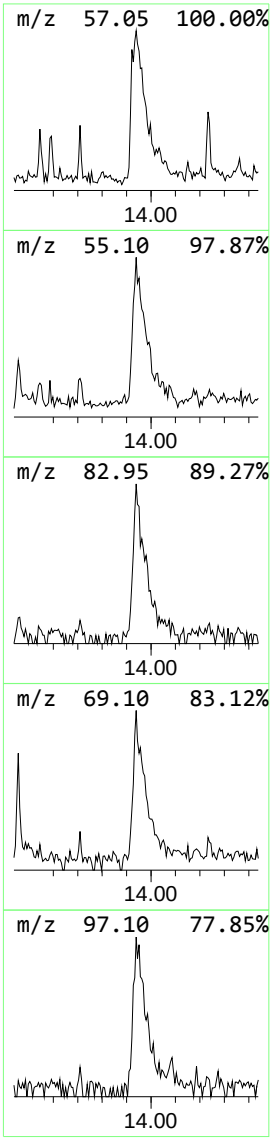
****

Peak Number 5 1-Heneicosanol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.939	6.67 ng	141400	Chrysene-d12	14.086

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol	312	C21H44O	015594-90-8	95
2	n-Nonadecanol-1	284	C19H40O	001454-84-8	94
3	1-Octadecanol	270	C18H38O	000112-92-5	94
4	Bromoacetic acid, hexadecyl ester	362	C18H35BrO2	005454-48-8	94
5	n-Heptadecanol-1	256	C17H36O	001454-85-9	91





Tentatively Identified Compound (LSC) summary

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					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2-Pentanone, 4-...	5.163	4.4	ng	124746	1	6.916	570237	20.0
Ethanol, 1-(2-b...	8.092	5.2	ng	199099	2	8.198	766627	20.0
Lenthionine	10.874	2.5	ng	110636	4	11.445	873133	20.0
2-Phenanthrenol...	13.457	2.8	ng	58647	5	14.086	424235	20.0
1-Heneicosanol	13.939	6.7	ng	141400	5	14.086	424235	20.0