LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080724\
Data File : BF138853.D
Acq On : 07 Aug 2024 20:37
Operator : RC/JU
Sample : P3430-04
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
931-K1-WP0-0-0.25-073124

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-BF073024.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF138853.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.146	3	9	15	rVB	1696720	2671264	100.00%	24.697%
2	3.387	215	220	235	rBV	10392	32676	1.22%	0.302%
3	5.063	500	505	517	rVB	26249	39271	1.47%	0.363%
4	5.469	569	574	595	rBV	493680	651732	24.40%	6.025%
5	6.481	741	746	756	rBV	318063	422411	15.81%	3.905%
6	6.840	802	807	812	rBV	224353	280393	10.50%	2.592%
7	7.404	896	903	908	rBV	722357	990540	37.08%	9.158%
8	7.663	942	947	959	rBV2	17244	33851	1.27%	0.313%
9	8.116	1019	1024	1030	rBV	284918	369475	13.83%	3.416%
10	8.434	1073	1078	1096	rVB	56836	86130	3.22%	0.796%
11	9.192	1201	1207	1212	rBV	1401697	1801177	67.43%	16.652%
12	9.869	1317	1322	1331	rVB	337308	417628	15.63%	3.861%
13	9.963	1331	1338	1343	rBV	19325	28698	1.07%	0.265%
14	10.663	1451	1457	1471	rBV	747714	980568	36.71%	9.066%
15	11.357	1570	1575	1580	rBV	317117	388165	14.53%	3.589%
16	11.880	1660	1664	1678	rBV3	25598	47153	1.77%	0.436%
17	12.939	1838	1844	1849	rBV	874476	1093286	40.93%	10.108%
18	13.839	1989	1997	2014	rBV2	23228	56478	2.11%	0.522%
19	13.998	2019	2024	2033	rVB	160273	213075	7.98%	1.970%
20	15.457	2266	2272	2279	rBV	142594	212294	7.95%	1.963%

Sum of corrected areas: 10816265

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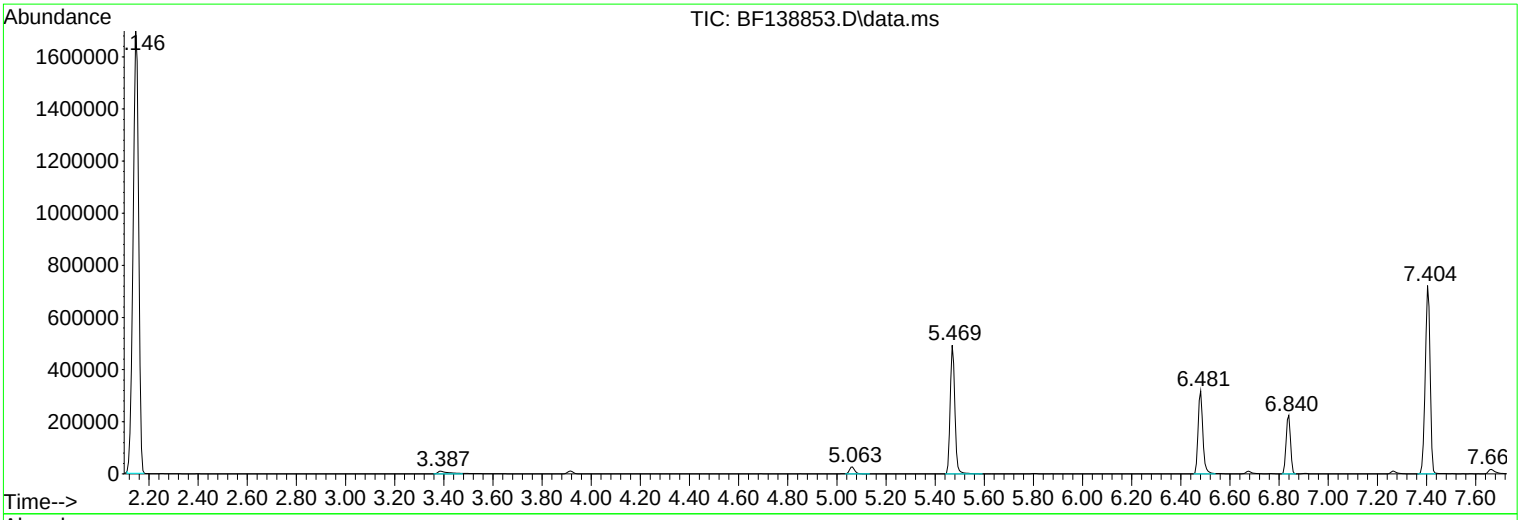
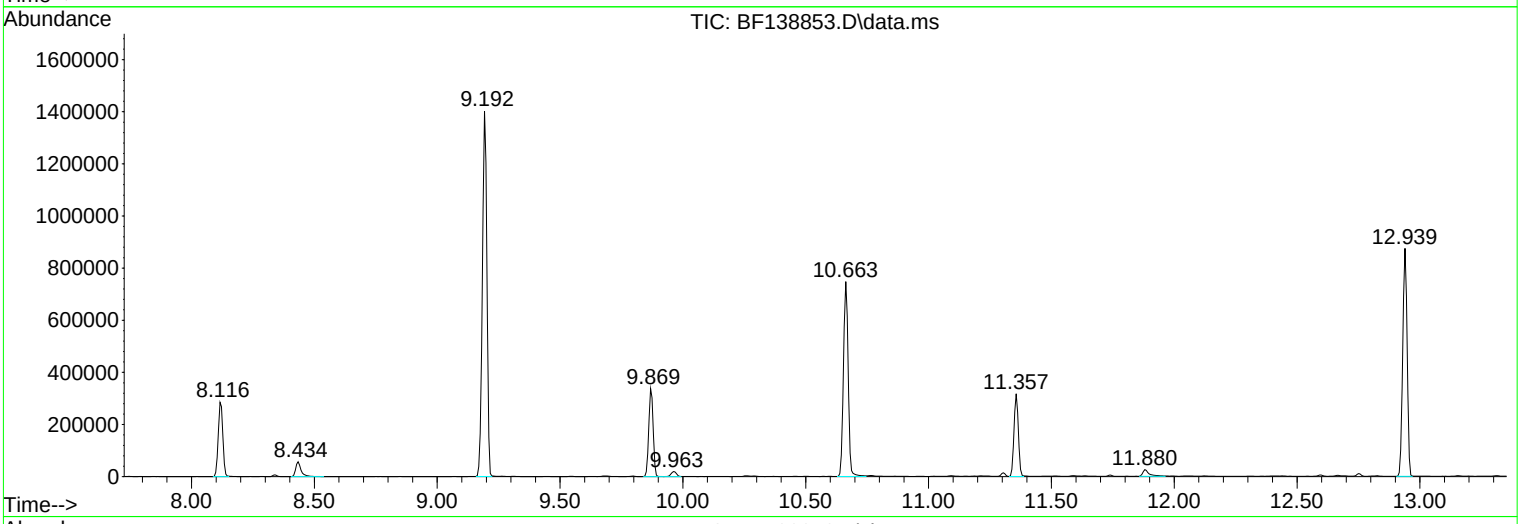
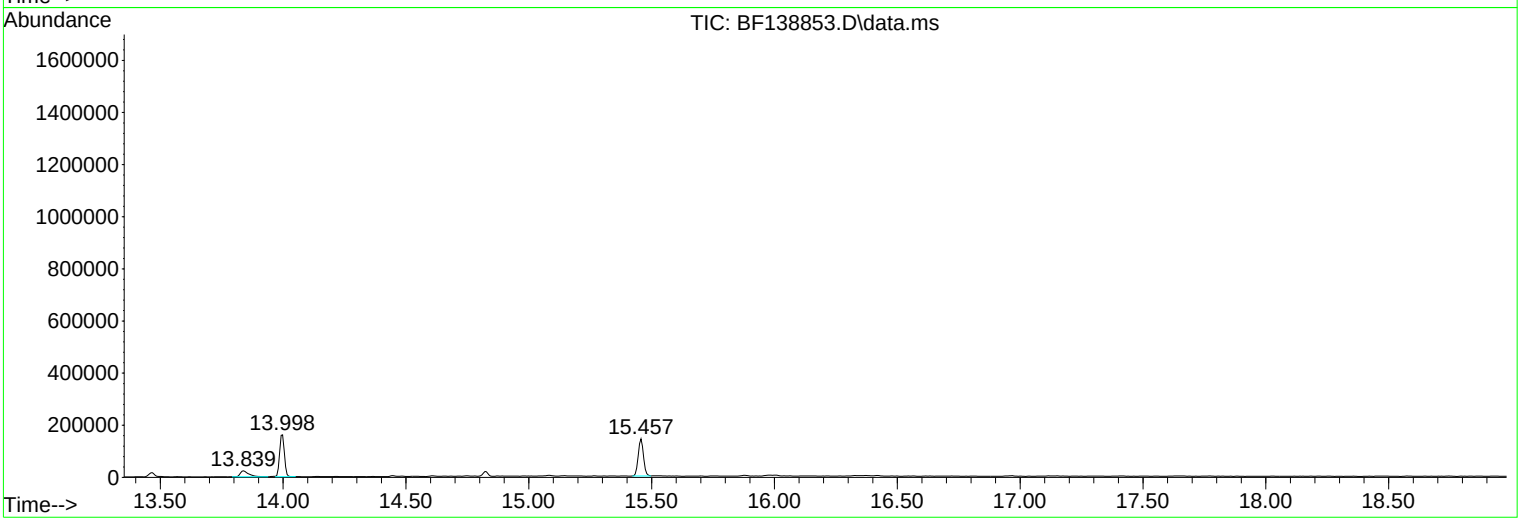
931-K1-WP0-0-0.25-073124

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF073024.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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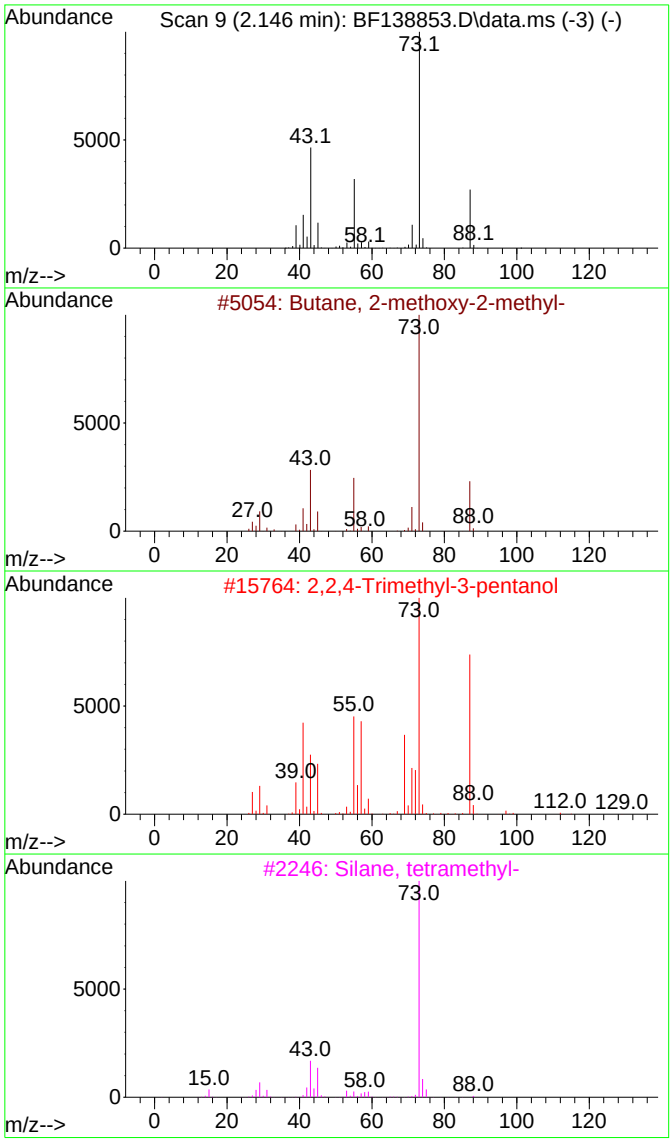
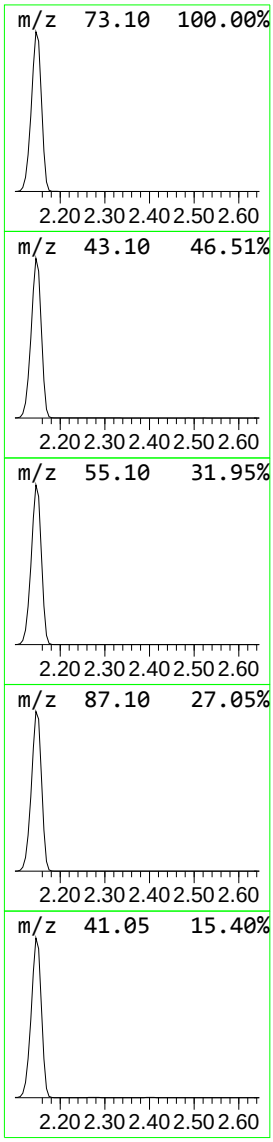
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.146	190.54 ng	2671260	1,4-Dichlorobenzene-d4	6.840

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	Silane, tetramethyl-	88	C4H12Si	000075-76-3	17
4	N-Ethylformamide	73	C3H7NO	000627-45-2	9
5	Borane, dimethoxy-	74	C2H7BO2	004542-61-4	9





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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF073024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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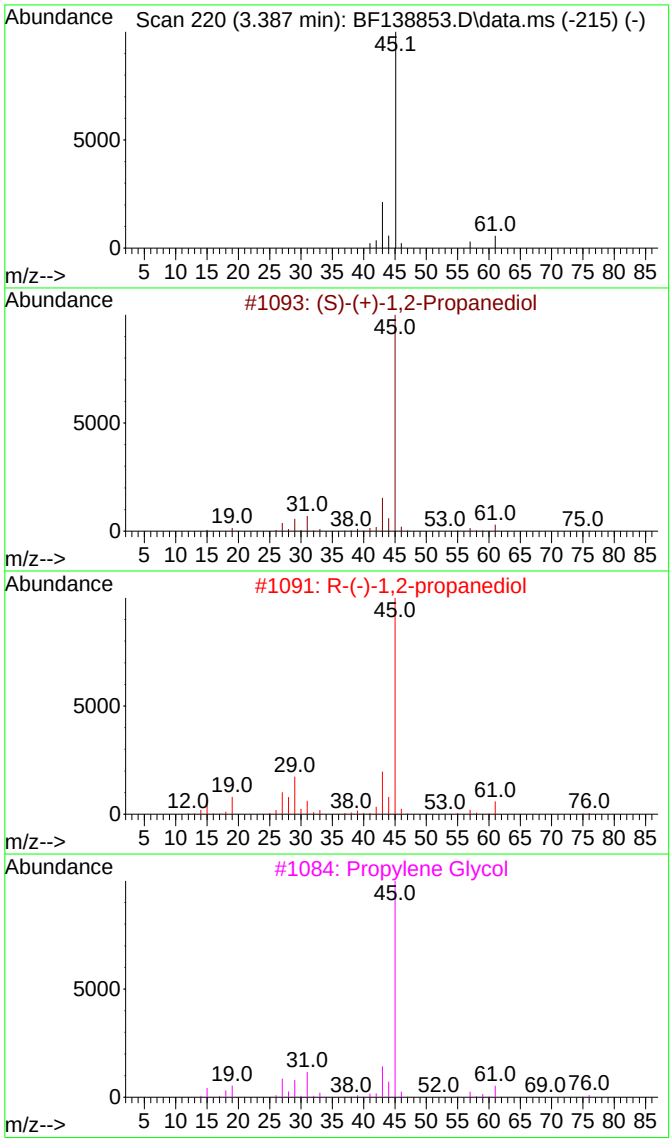
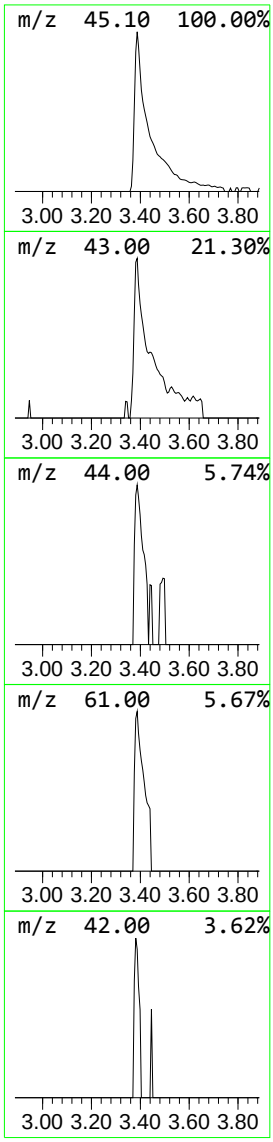
****

Peak Number 2 (S)-(+)-1,2-Propanediol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.387	2.33 ng	32676	1,4-Dichlorobenzene-d4	6.840

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	64
2	R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	9
3	Propylene Glycol	76	C3H8O2	000057-55-6	9
4	Isopropyl Alcohol	60	C3H8O	000067-63-0	9
5	Formamide	45	CH3NO	000075-12-7	5





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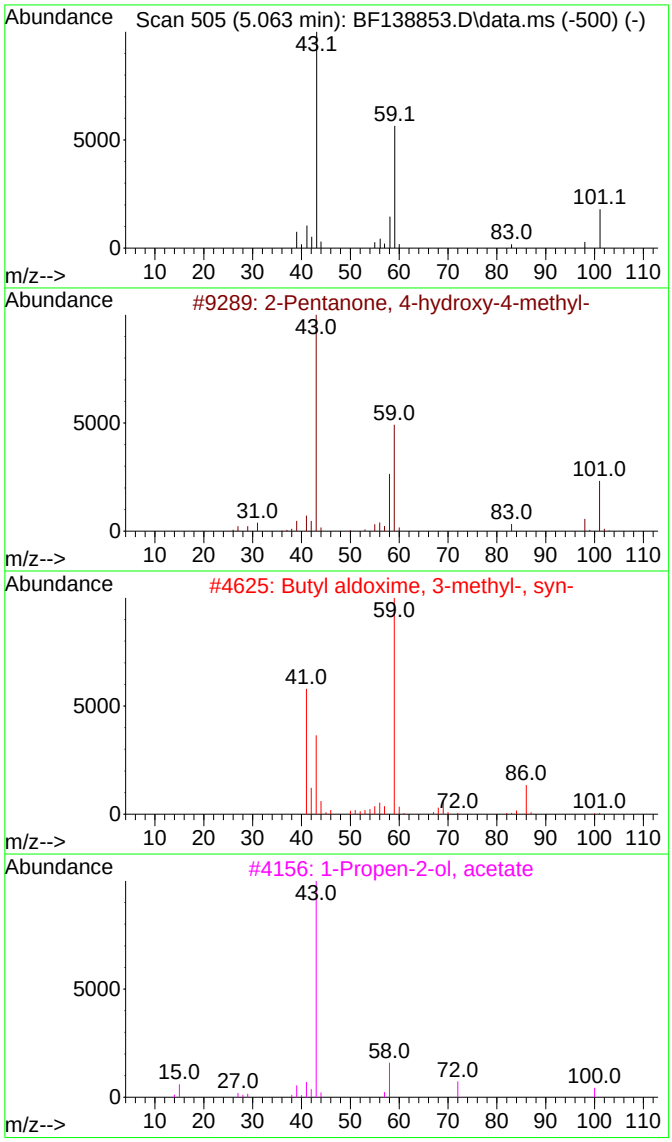
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF073024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

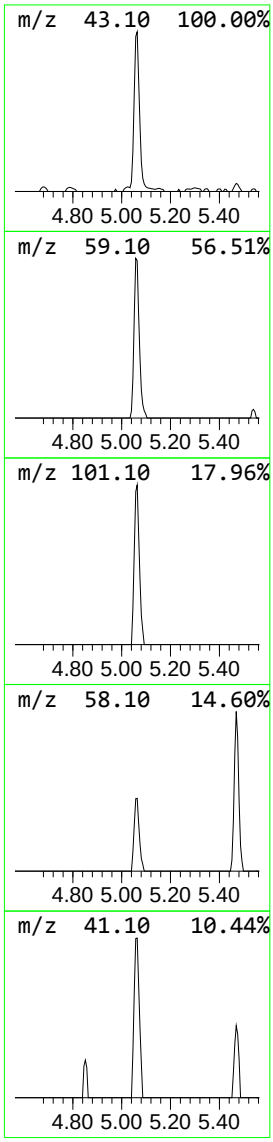
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.063	2.80 ng	39271	1,4-Dichlorobenzene-d4	6.840

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	37
3	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5	Diacetamide	101	C4H7NO2	000625-77-4	9





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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF073024.M
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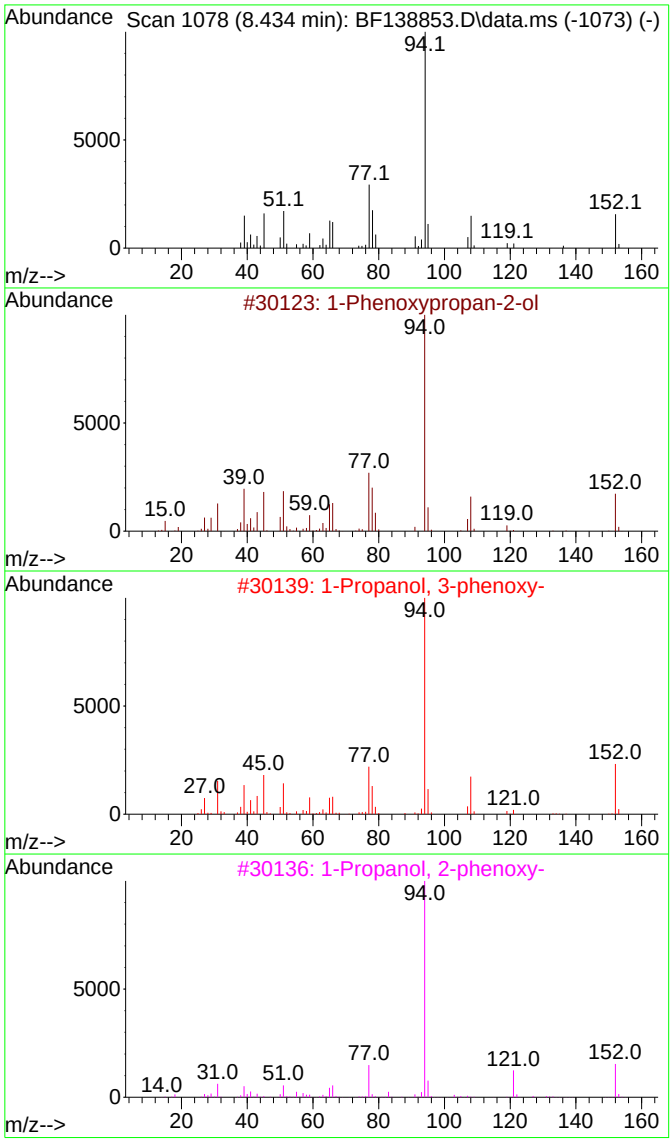
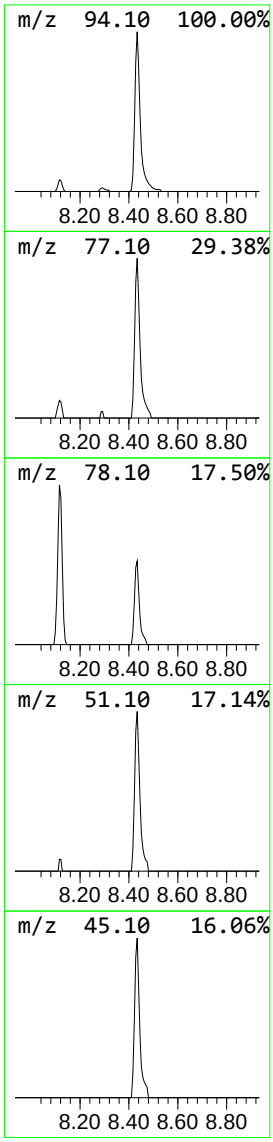
****

Peak Number 4 1-Phenoxypropan-2-ol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.434	4.66 ng	86130	Naphthalene-d8	8.116

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Phenoxypropan-2-ol	152	C9H12O2	000770-35-4	96
2	1-Propanol, 3-phenoxy-	152	C9H12O2	006180-61-6	87
3	1-Propanol, 2-phenoxy-	152	C9H12O2	004169-04-4	59
4	Ethanol, 2-phenoxy-	138	C8H10O2	000122-99-6	59
5	Benzene, (1,1-dimethylethoxy)-	150	C10H14O	006669-13-2	53





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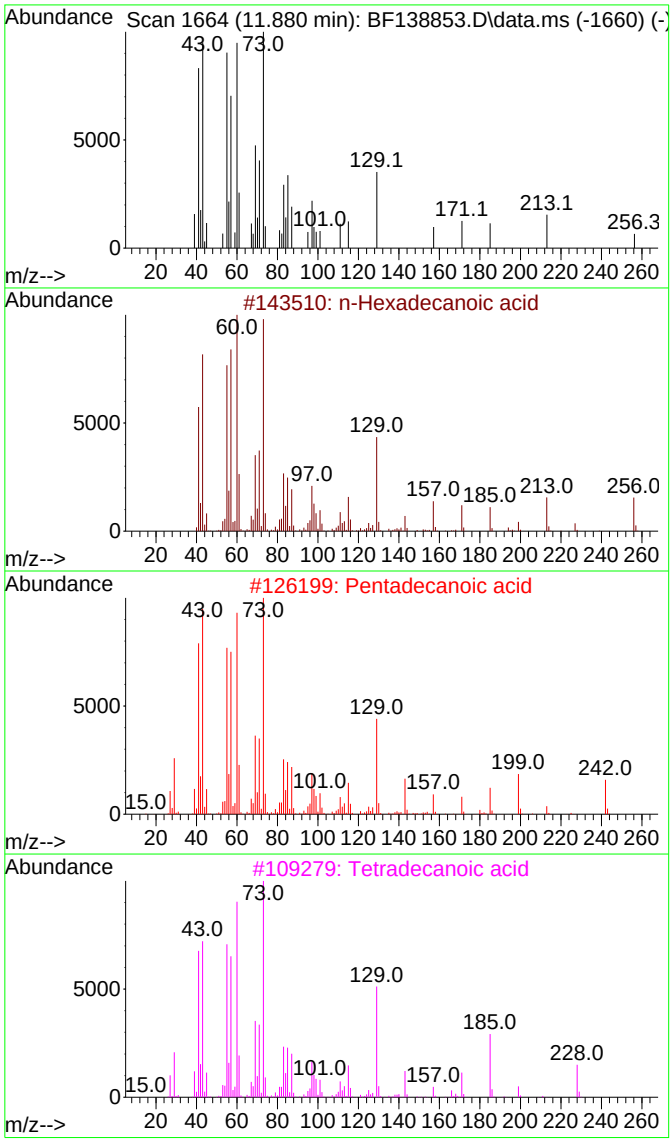
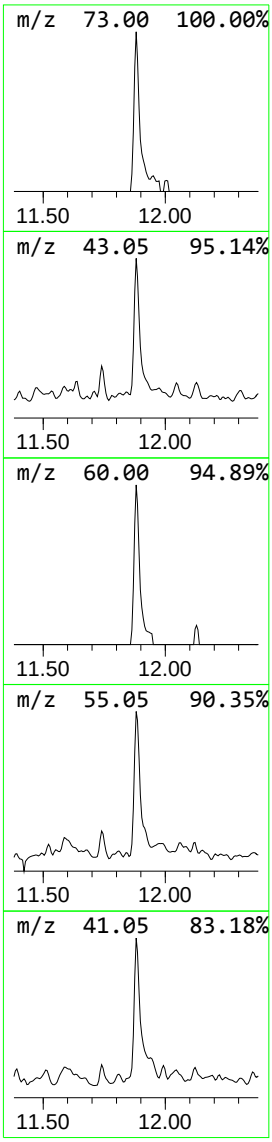
****

Peak Number 5 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.880	2.43 ng	47153	Phenanthrene-d10	11.357

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	91
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	80
4	n-Decanoic acid	172	C10H20O2	000334-48-5	59
5	Tridecanoic acid	214	C13H26O2	000638-53-9	53





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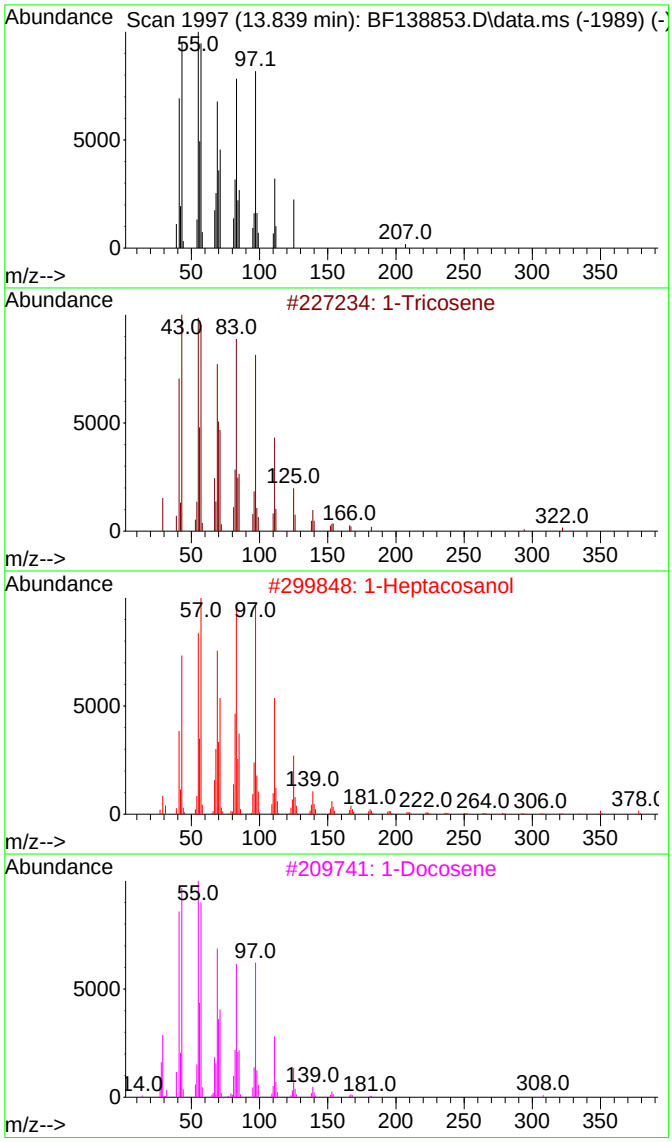
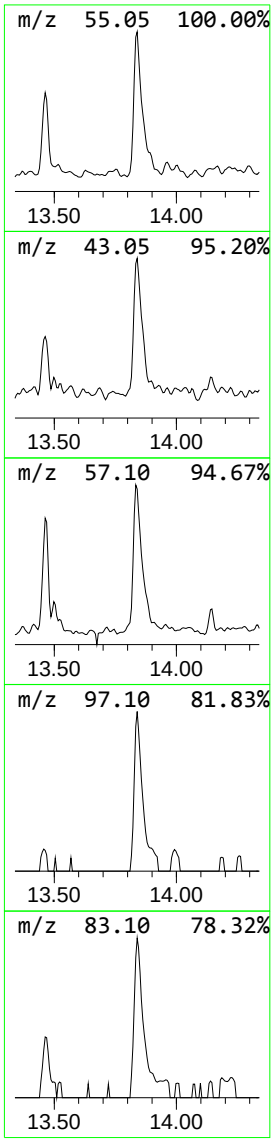
****

Peak Number 6 1-Tricosene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.839	5.30 ng	56478	Chrysene-d12	13.998

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Tricosene	322	C23H46	018835-32-0	91
2	1-Heptacosanol	396	C27H56O	002004-39-9	91
3	1-Docosene	308	C22H44	001599-67-3	91
4	Heptacosyl acetate	438	C29H58O2	1000351-78-2	91
5	Behenic alcohol	326	C22H46O	000661-19-8	91





Tentatively Identified Compound (LSC) summary

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TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Butane, 2-metho...	2.146	190.5	ng	2671260	1	6.840	280393	20.0
(S)-(+)-1,2-Pro...	3.387	2.3	ng	32676	1	6.840	280393	20.0
2-Pentanone, 4-...	5.063	2.8	ng	39271	1	6.840	280393	20.0
1-Phenoxypropan...	8.434	4.7	ng	86130	2	8.116	369475	20.0
n-Hexadecanoic ...	11.880	2.4	ng	47153	4	11.357	388165	20.0
1-Tricosene	13.839	5.3	ng	56478	5	13.998	213075	20.0