LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080324\
Data File : BF138776.D
Acq On : 03 Aug 2024 18:19
Operator : RC/JU
Sample : P3448-13
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP7

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: BF138776.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.134	3	7	19	rVB	651810	979404	86.39%	12.007%
2	3.381	214	219	232	rBV	10077	28417	2.51%	0.348%
3	5.069	501	506	515	rVB	46038	69257	6.11%	0.849%
4	5.475	570	575	593	rBV	724964	933413	82.33%	11.443%
5	6.487	741	747	762	rBV	729928	965254	85.14%	11.834%
6	6.681	775	780	788	rBV2	6855	12489	1.10%	0.153%
7	6.845	803	808	813	rBB	217421	262621	23.16%	3.220%
8	7.410	898	904	915	rBV	485344	636271	56.12%	7.800%
9	7.663	943	947	952	rBV	15499	19784	1.75%	0.243%
10	8.122	1020	1025	1037	rVB	273867	350207	30.89%	4.293%
11	8.439	1074	1079	1091	rBV	28997	46148	4.07%	0.566%
12	9.198	1202	1208	1213	rBV	928389	1133745	100.00%	13.899%
13	9.875	1318	1323	1334	rVB	303681	388491	34.27%	4.763%
14	9.969	1334	1339	1347	rBV	22825	32588	2.87%	0.400%
15	10.669	1453	1458	1471	rBV	466154	588036	51.87%	7.209%
16	11.363	1571	1576	1584	rBV	274149	345430	30.47%	4.235%
17	11.892	1661	1666	1674	rBV4	17252	31034	2.74%	0.380%
18	12.951	1840	1846	1850	rBV	600034	777043	68.54%	9.526%
19	13.857	1993	2000	2015	rBV2	25935	67719	5.97%	0.830%
20	14.004	2020	2025	2033	rVB	166012	213310	18.81%	2.615%
21	15.474	2269	2275	2283	rBV	162225	248519	21.92%	3.047%
22	16.021	2359	2368	2379	rBV	6662	27644	2.44%	0.339%

Sum of corrected areas: 8156824

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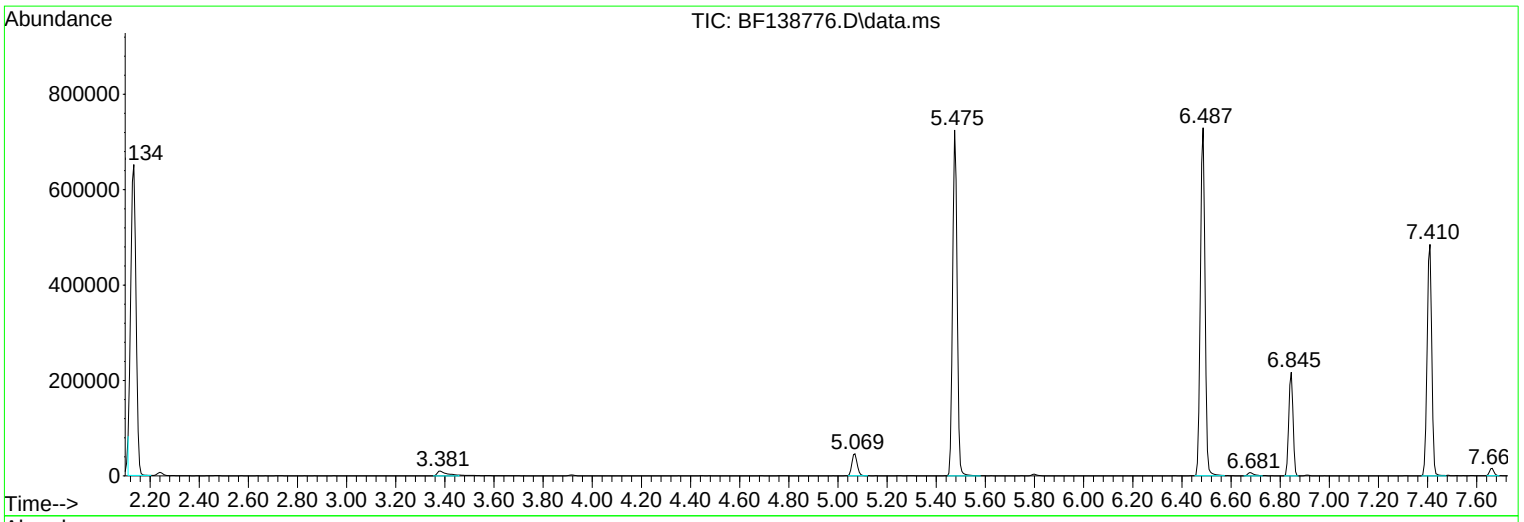
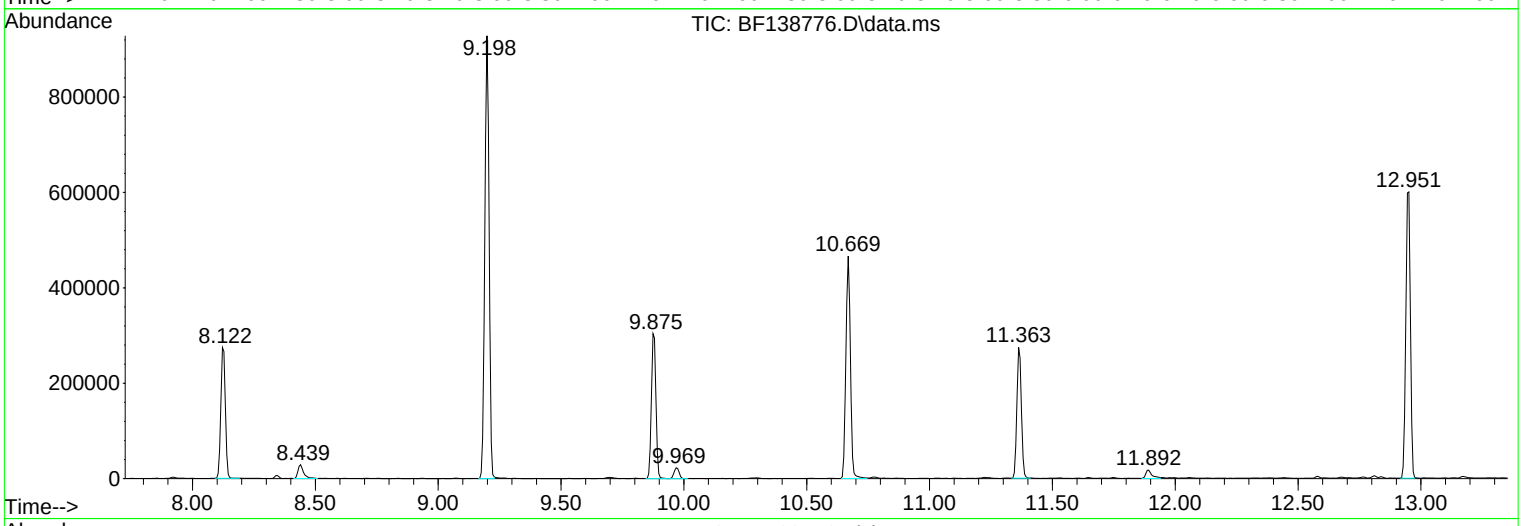
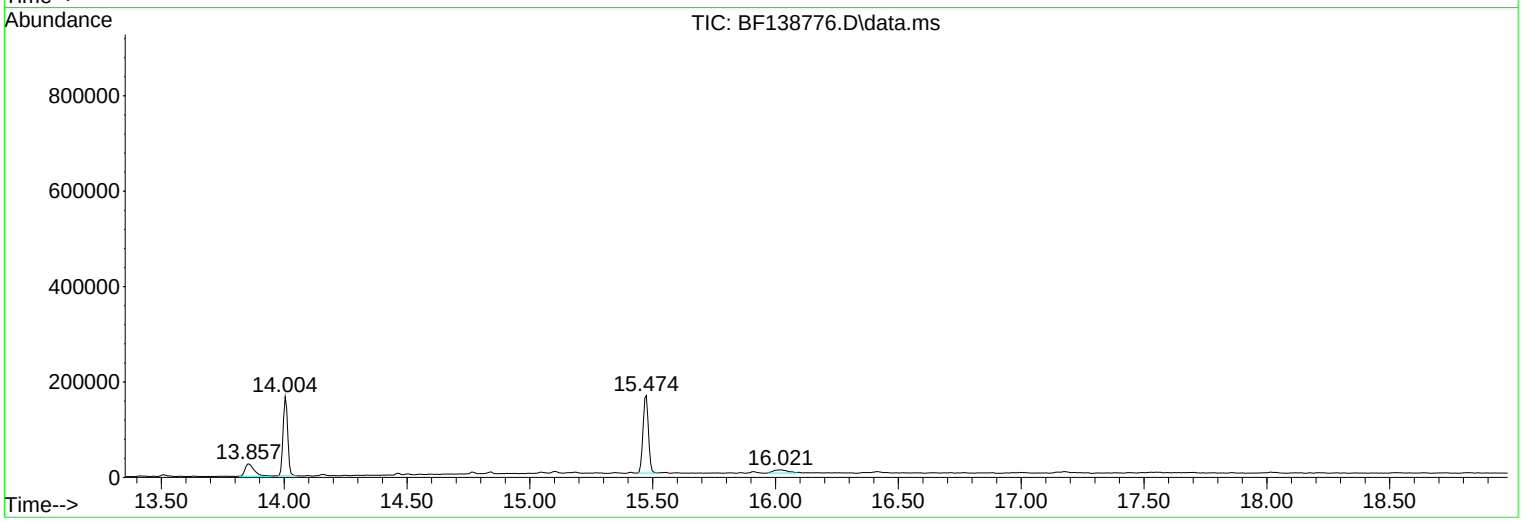
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF073024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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







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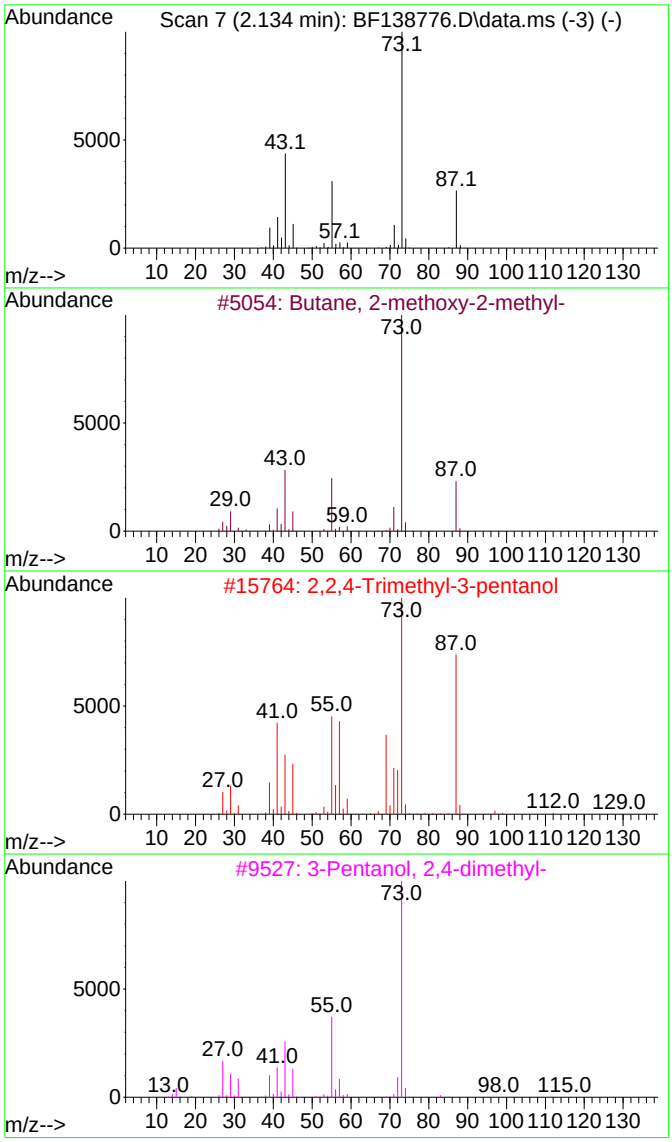
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

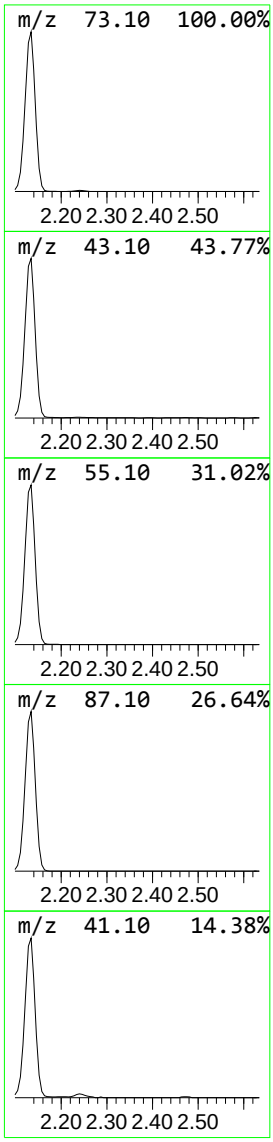
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.134	74.59 ng	979404	1,4-Dichlorobenzene-d4	6.845

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	3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	37
4	Silane, tetramethyl-	88	C4H12Si	000075-76-3	35
5	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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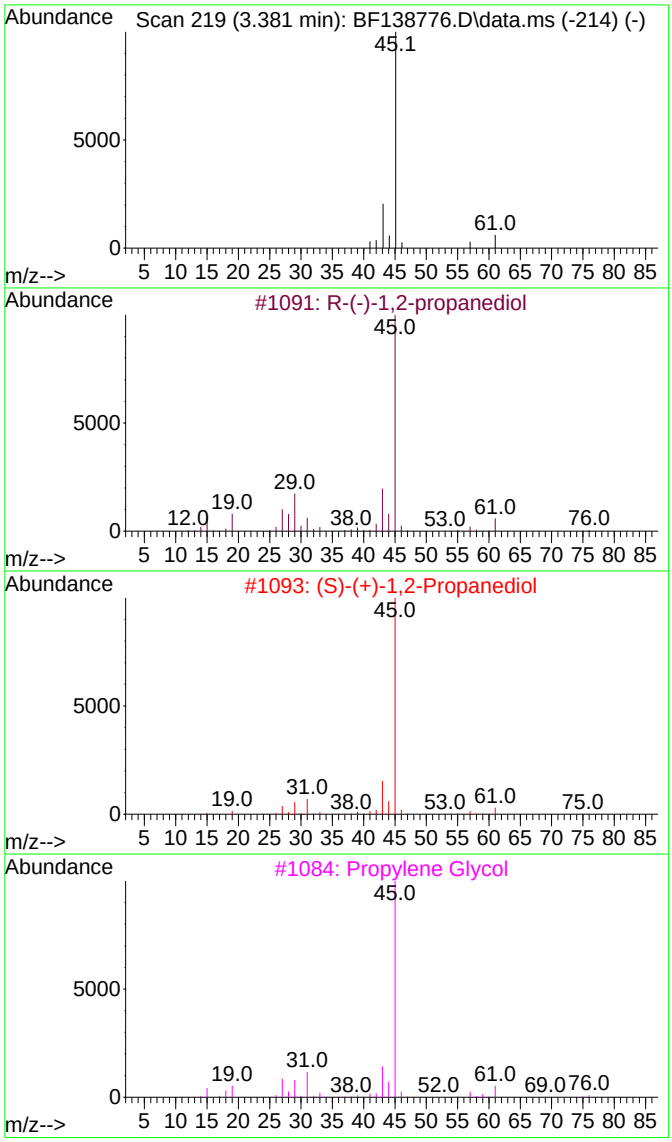
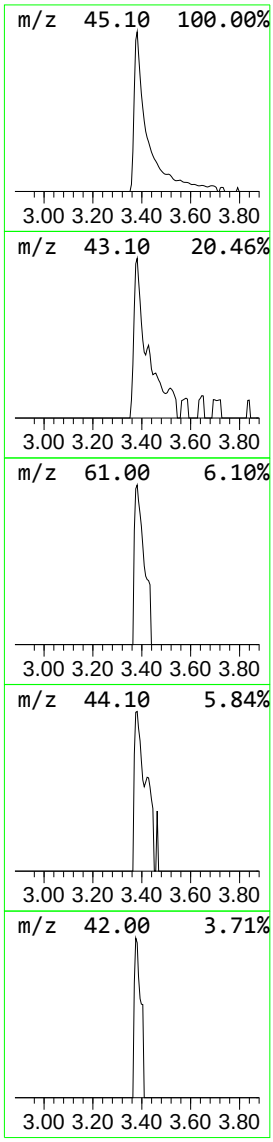
Peak Number 2 R-(-)-1,2-propanediol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.381	2.16 ng	28417	1,4-Dichlorobenzene-d4	6.845

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	64
2	(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	64
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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Misc :
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Instrument :
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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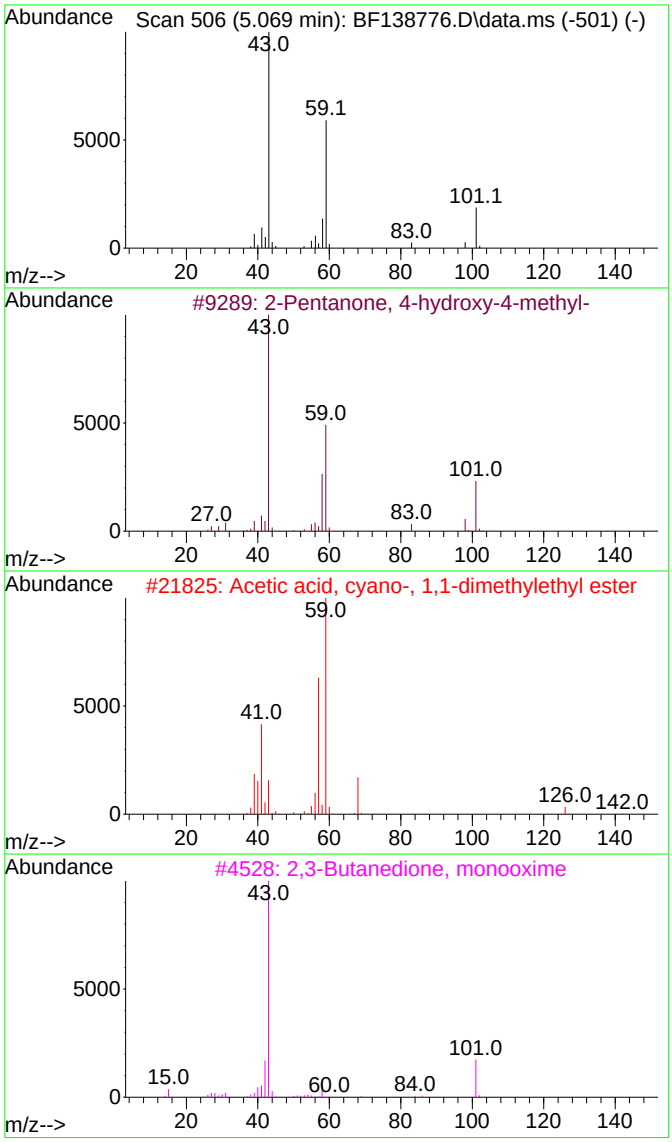
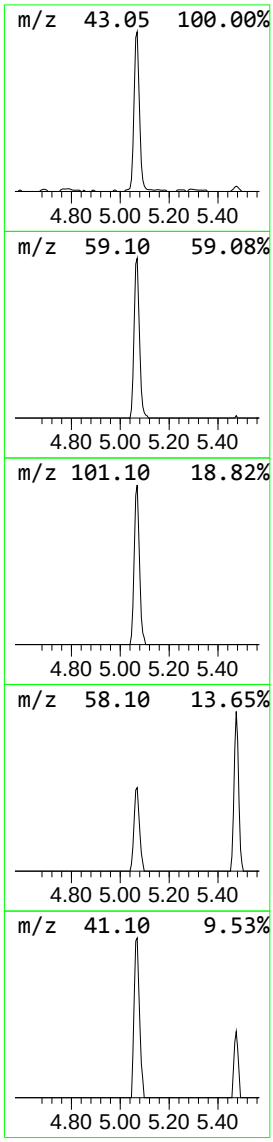
Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.069	5.27 ng	69257	1,4-Dichlorobenzene-d4	6.845

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12
5	2-Propyn-1-ol, acetate	98	C5H6O2	000627-09-8	9





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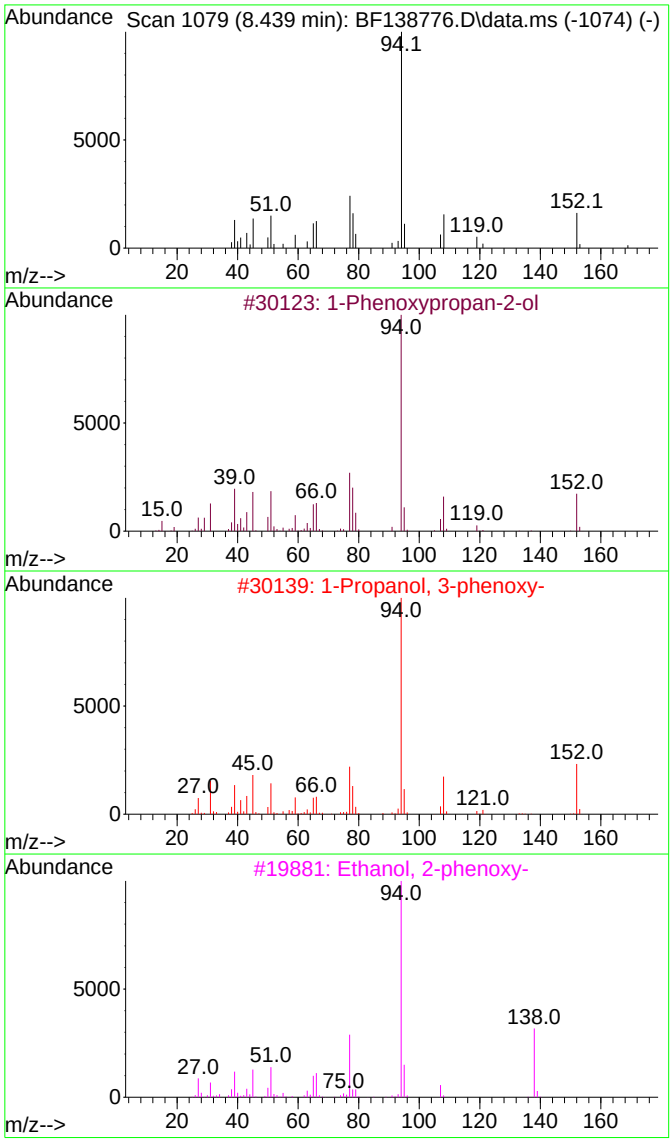
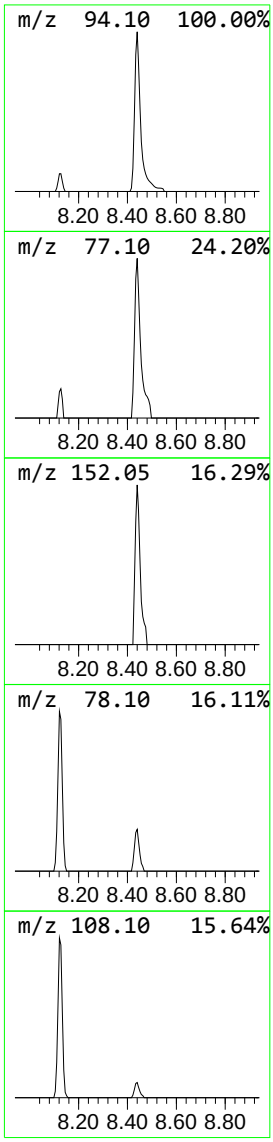
Peak Number 4 1-Phenoxypropan-2-ol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.439	2.64 ng	46148	Naphthalene-d8	8.122

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	90
3	Ethanol, 2-phenoxy-	138	C8H10O2	000122-99-6	64
4	1-Propanol, 2-phenoxy-	152	C9H12O2	004169-04-4	64
5	Carbonic acid, neopentyl phenyl ...	208	C12H16O3	013183-19-2	59





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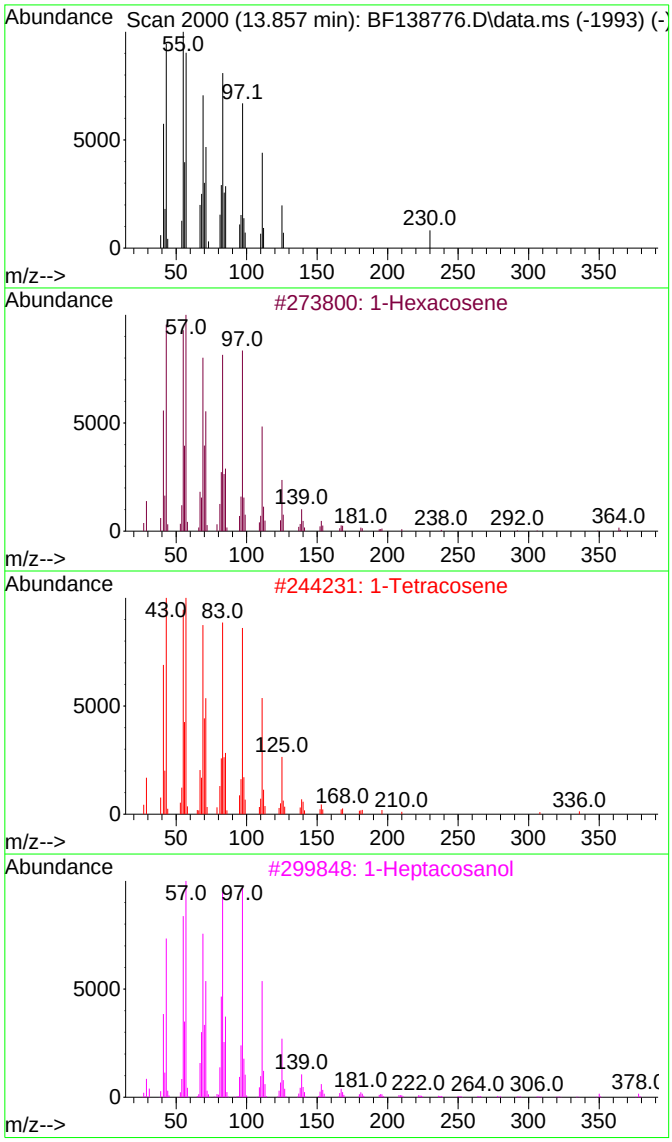
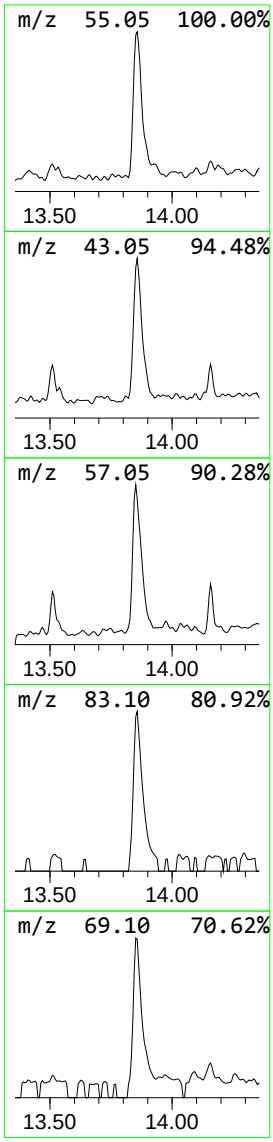
Peak Number 5 1-Hexacosene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.857	6.35 ng	67719	Chrysene-d12	14.004

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexacosene	364	C26H52	018835-33-1	95
2	1-Tetracosene	336	C24H48	010192-32-2	94
3	1-Heptacosanol	396	C27H56O	002004-39-9	93
4	Octacosanol	410	C28H58O	000557-61-9	91
5	1-Docosene	308	C22H44	001599-67-3	90





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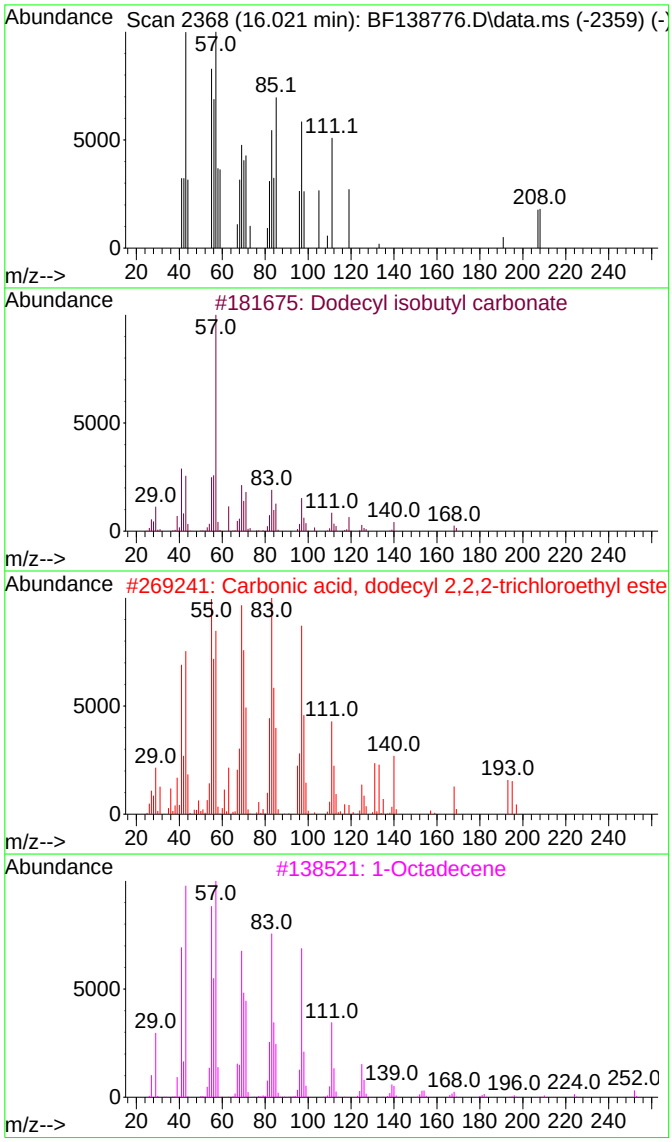
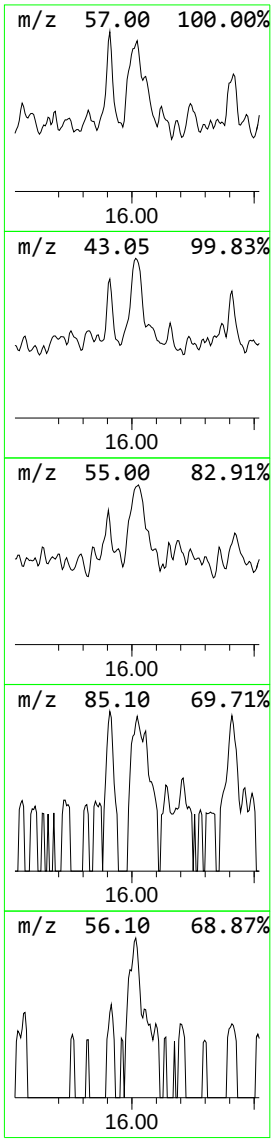
Peak Number 6 Dodecyl isobutyl carbonate Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.021	2.22 ng	27644	Perylene-d12	15.474

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dodecyl isobutyl carbonate	286	C17H34O3	959067-22-2	64
2	Carbonic acid, dodecyl 2,2,2-tri...	360	C15H27Cl3O3	1000314-55-8	50
3	1-Octadecene	252	C18H36	000112-88-9	50
4	Decyl isobutyl carbonate	258	C15H30O3	959226-07-4	50
5	Hexadecane, 1,1-bis(dodecyloxy)-	595	C40H82O2	056554-64-4	49





Tentatively Identified Compound (LSC) summary

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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...	2.134	74.6	ng	979404	1	6.845	262621	20.0
R-(-)-1,2-propa...	3.381	2.2	ng	28417	1	6.845	262621	20.0
2-Pentanone, 4-...	5.069	5.3	ng	69257	1	6.845	262621	20.0
1-Phenoxypropan...	8.439	2.6	ng	46148	2	8.122	350207	20.0
1-Hexacosene	13.857	6.3	ng	67719	5	14.004	213310	20.0
Dodecyl isobuty...	16.021	2.2	ng	27644	6	15.474	248519	20.0