LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062221\
Data File : BG049049.D
Acq On : 22 Jun 2021 17:14
Operator : CG/JU
Sample : M2773-10
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-10

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_G\METHODS\8270-BG061121.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG049049.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.158	15	20	29	rBV	65845	131133	6.32%	1.278%
2	3.234	29	33	41	rVB	22533	36961	1.78%	0.360%
3	5.191	361	366	374	rVB	27609	48494	2.34%	0.473%
4	5.661	438	446	456	rBV	450063	747224	35.99%	7.284%
5	7.265	711	719	733	rBV	454708	812311	39.12%	7.919%
6	8.111	856	863	870	rBV	109048	192475	9.27%	1.876%
7	9.274	1053	1061	1070	rBV	285977	524281	25.25%	5.111%
8	10.690	1296	1302	1311	rBV	99565	171217	8.25%	1.669%
9	10.931	1335	1343	1353	rVB	144543	269172	12.96%	2.624%
10	13.375	1748	1759	1766	rBV	717372	1172493	56.47%	11.430%
11	14.750	1987	1993	2000	rVB	246287	390419	18.80%	3.806%
12	16.237	2240	2246	2259	rBV	738589	1117692	53.83%	10.895%
13	17.500	2454	2461	2466	rBV	345945	546333	26.31%	5.326%
14	17.547	2466	2469	2473	rVB2	31080	41916	2.02%	0.409%
15	18.381	2604	2611	2615	rBV3	85171	119172	5.74%	1.162%
16	19.450	2785	2793	2799	rBV7	14159	34002	1.64%	0.331%
17	19.550	2804	2810	2815	rVB	63572	96053	4.63%	0.936%
18	19.644	2822	2826	2831	rBV2	38354	51308	2.47%	0.500%
19	19.909	2862	2871	2877	rBV	60749	112025	5.40%	1.092%
20	20.109	2897	2905	2913	rBV	1538562	2076241	100.00%	20.239%
21	21.413	3123	3127	3138	rBV3	77407	148016	7.13%	1.443%
22	21.789	3182	3191	3196	rBV	353675	637786	30.72%	6.217%
23	22.635	3328	3335	3343	rBV	16720	48502	2.34%	0.473%
24	23.540	3483	3489	3496	rVB2	41068	80163	3.86%	0.781%
25	24.045	3571	3575	3580	rBV8	14986	36754	1.77%	0.358%
26	24.186	3593	3599	3604	rBV10	11805	24220	1.17%	0.236%
27	25.114	3747	3757	3768	rBV2	188759	592029	28.51%	5.771%

Sum of corrected areas: 10258392

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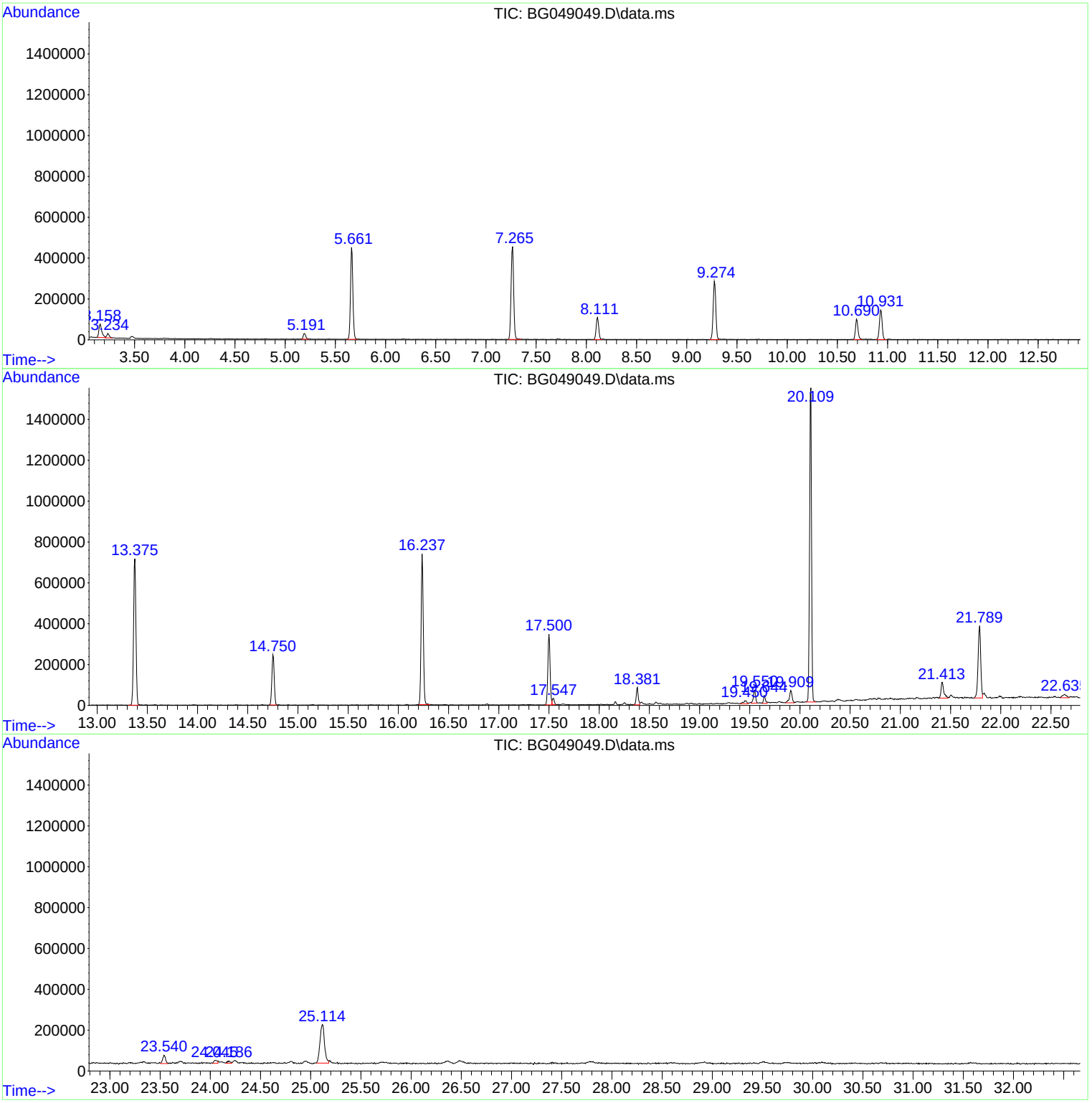
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG061121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P



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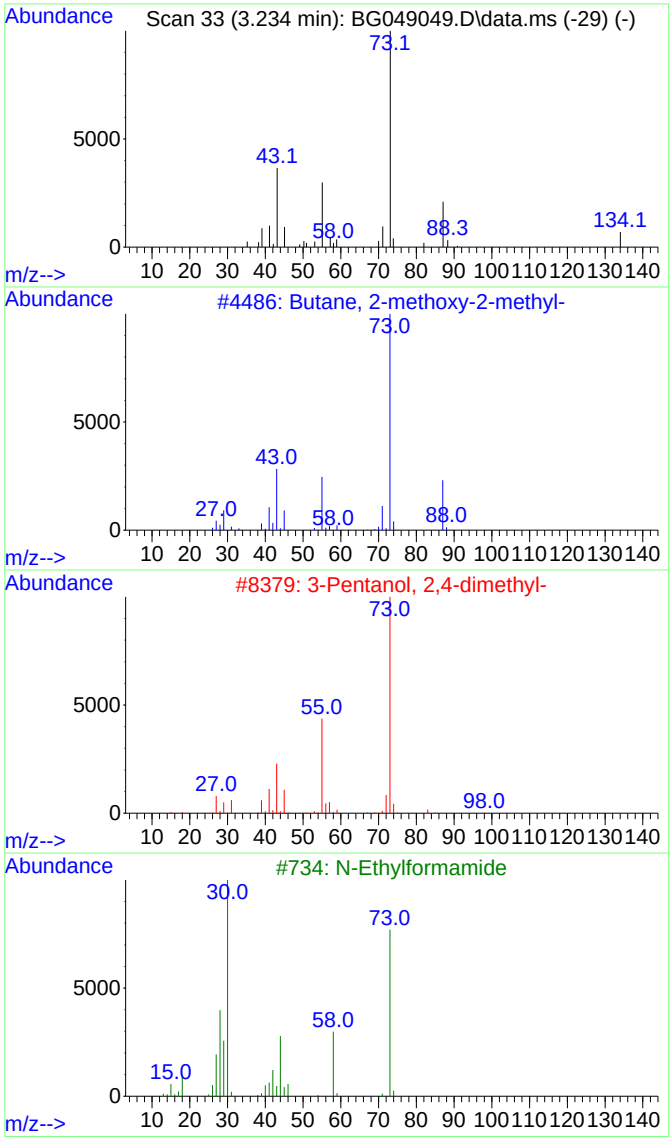
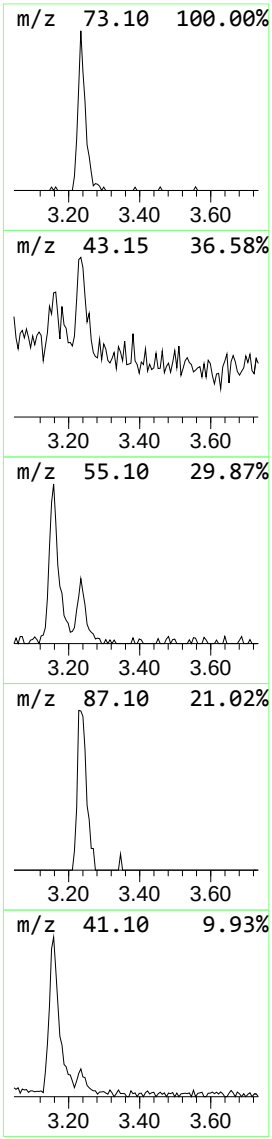
****

Peak Number 2 Butane, 2-methoxy-2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.234	3.84 ng	36961	1,4-Dichlorobenzene-d4	8.111

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	56
2	3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	25
3	N-Ethylformamide	73	C3H7NO	000627-45-2	9
4	N-(2-Thioethyl) N'-methyl urea	134	C4H10N2OS	072545-68-7	9
5	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	9





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

TIC Library : C:\Database\NIST11.L
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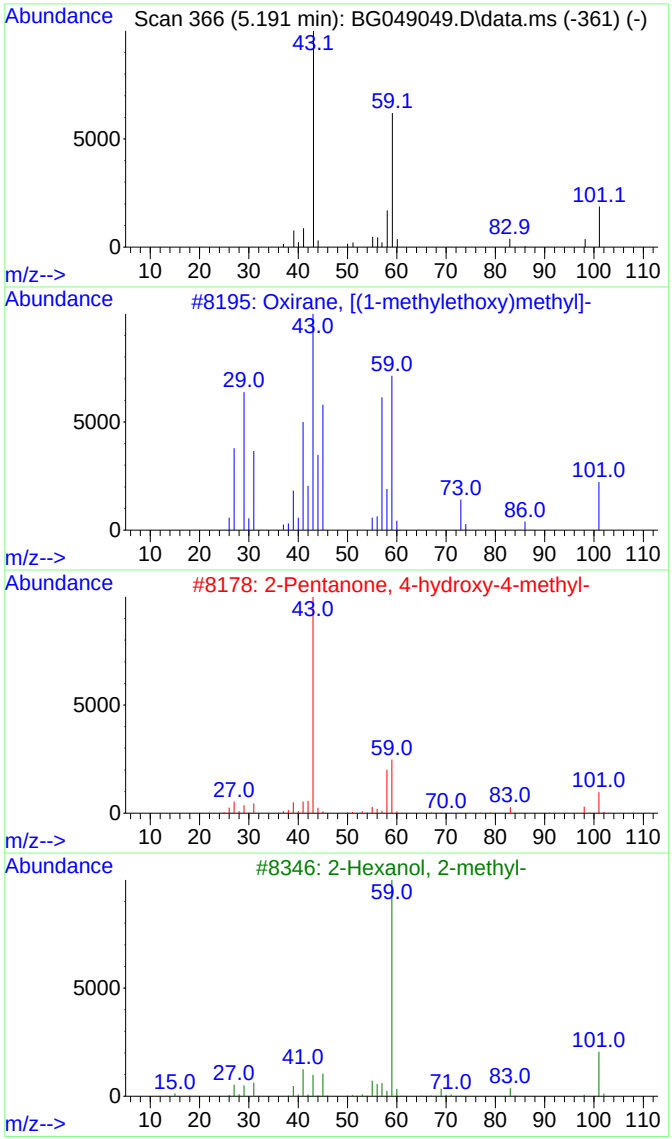
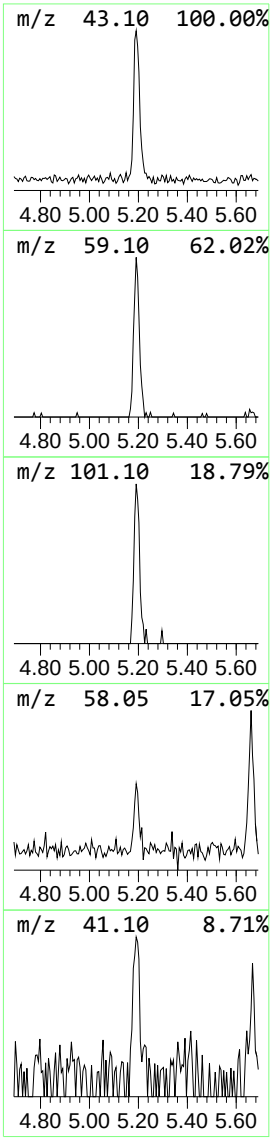
****
Peak Number 3 Oxirane, [(1-methylethoxy)m... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.191	5.04 ng	48494	1,4-Dichlorobenzene-d4	8.111

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oxirane, [(1-methylethoxy)methyl]-	116	C6H12O2	004016-14-2	50
2	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	45
3	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	40
4	5-Hexen-2-one	98	C6H10O	000109-49-9	10
5	2-Propyn-1-ol, acetate	98	C5H6O2	000627-09-8	9





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ClientSampleId : SB-10

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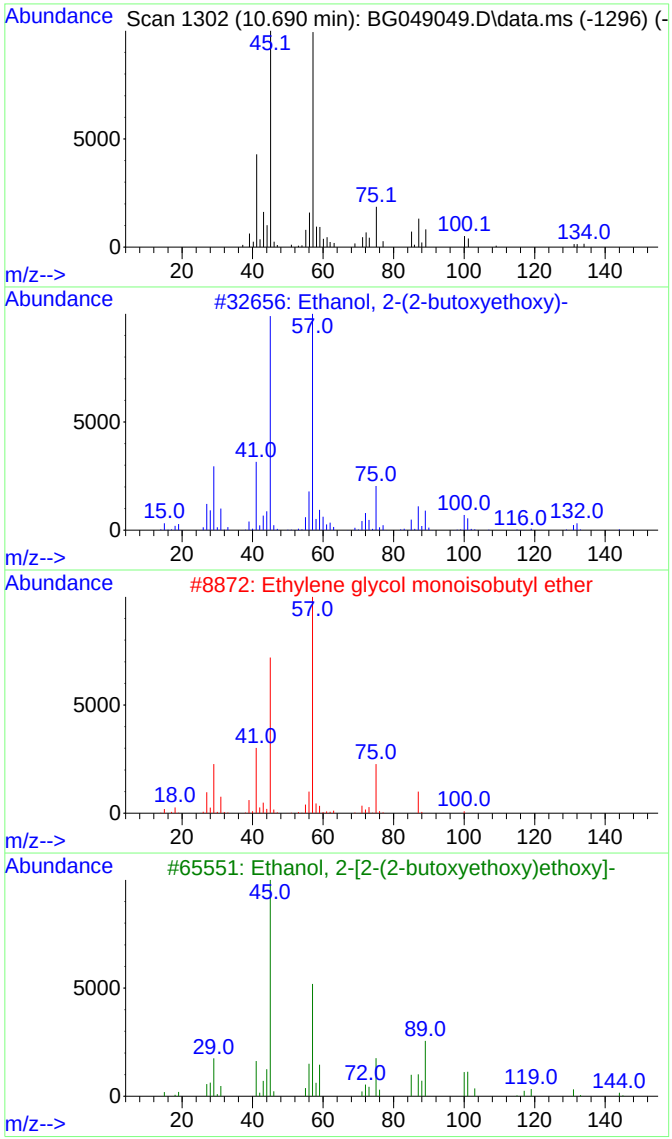
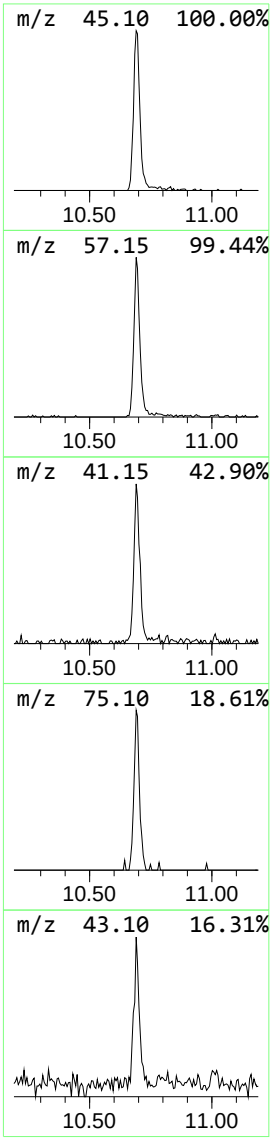
****
Peak Number 4 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.690	12.72 ng	171217	Naphthalene-d8	10.931

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	83
2	Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	64
3	Ethanol, 2-[2-(2-butoxyethoxy)et...	206	C10H22O4	000143-22-6	45
4	Propane, 2-ethoxy-	88	C5H12O	000625-54-7	43
5	Butane, 1-methoxy-	88	C5H12O	000628-28-4	43





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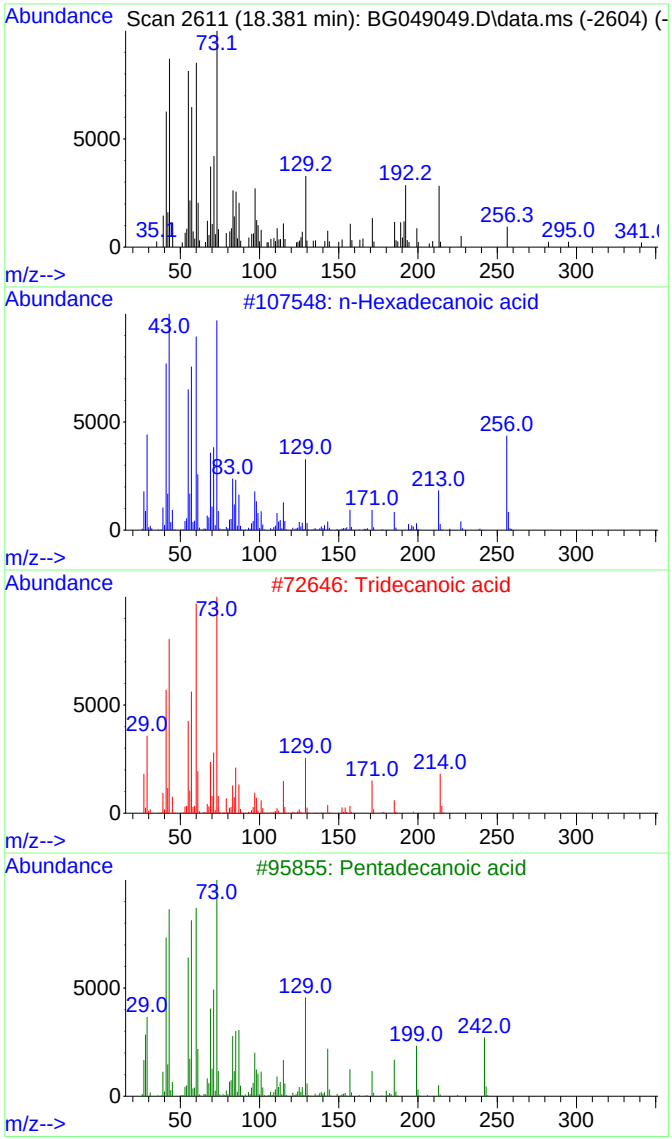
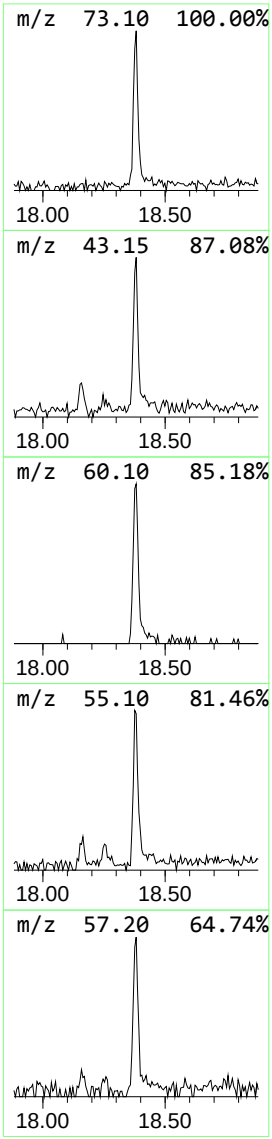
Peak Number 5 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.381	4.36 ng	119172	Phenanthrene-d10	17.500

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	97
2	Tridecanoic acid	214	C13H26O2	000638-53-9	89
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	74
4	Octadecanoic acid	284	C18H36O2	000057-11-4	68
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	64





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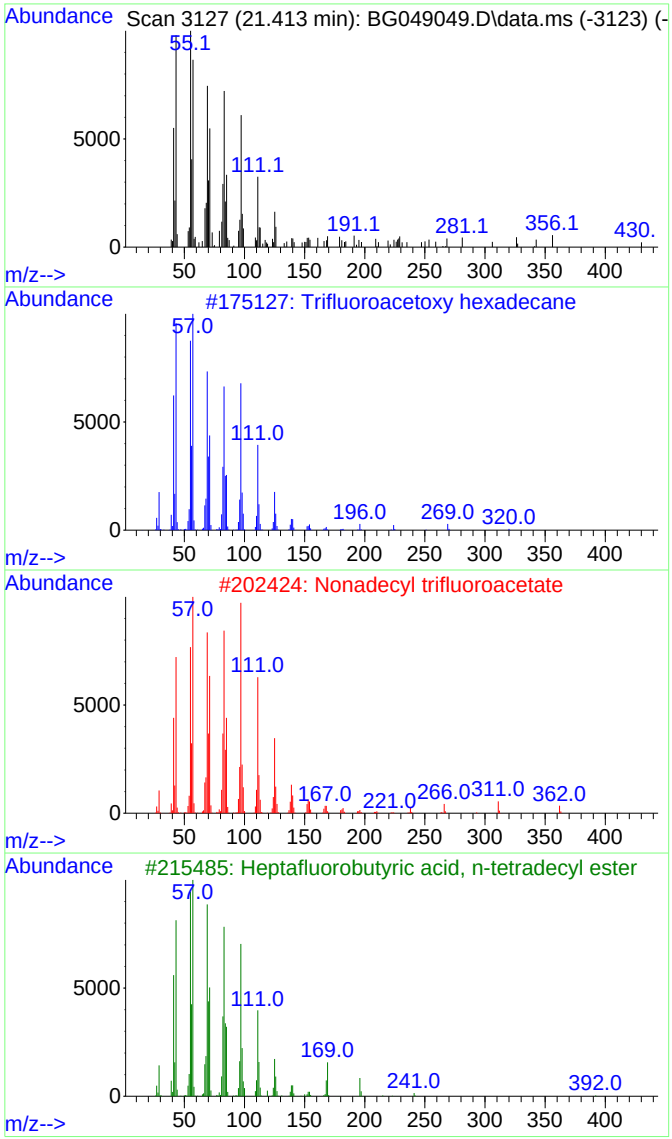
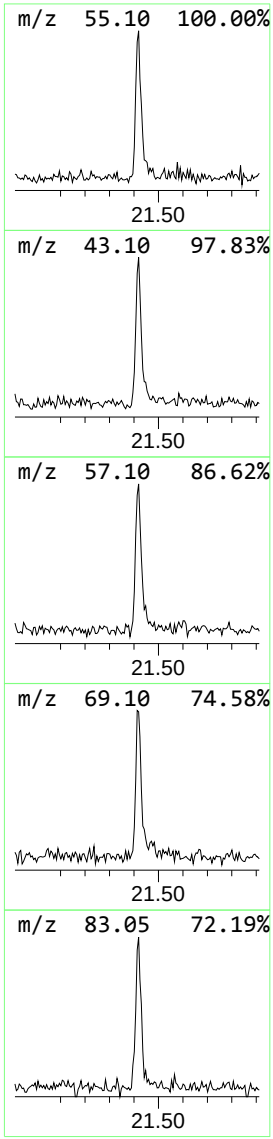
****

Peak Number 6 Trifluoroacetoxy hexadecane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.413	4.64 ng	148016	Chrysene-d12	21.789

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	93
2	Nonadecyl trifluoroacetate	380	C21H39F3O2	1000351-76-3	91
3	Heptafluorobutyric acid, n-tetra...	410	C18H29F7O2	007365-36-8	90
4	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	90
5	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	90





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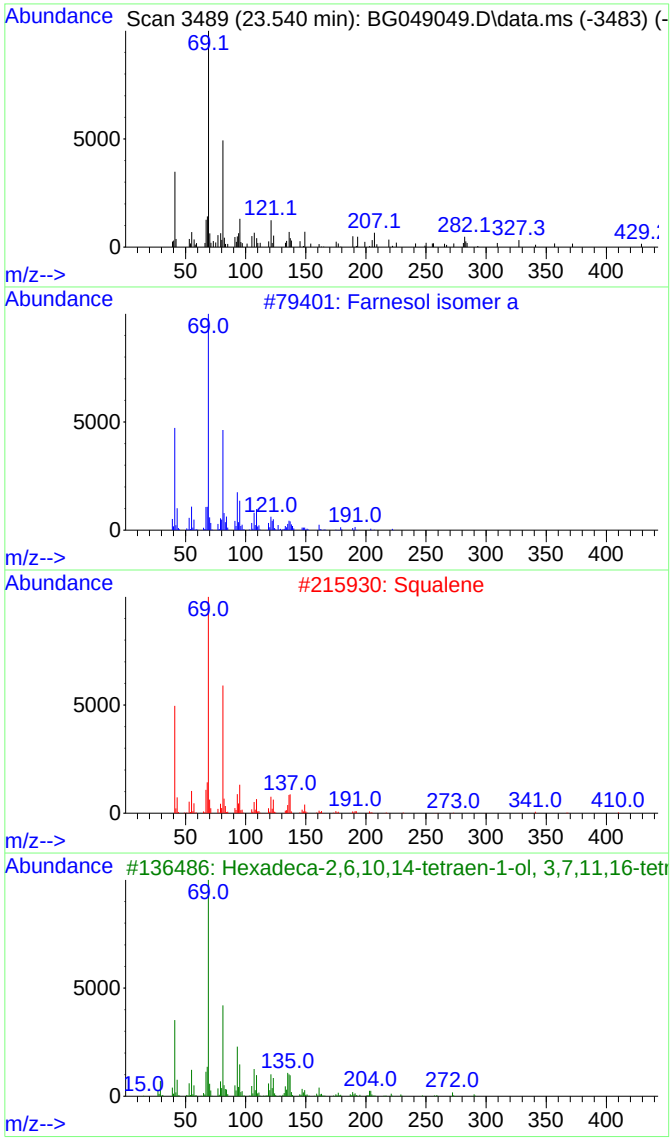
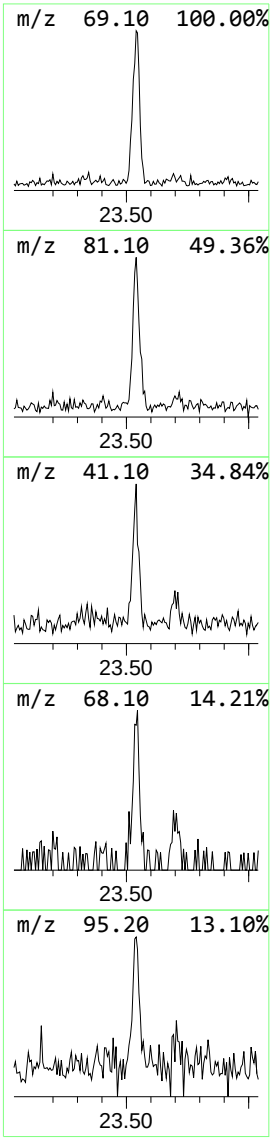
****

Peak Number 7 Farnesol isomer a Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.540	2.71 ng	80163	Perylene-d12	25.114

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Farnesol isomer a	222	C15H26O	1000108-92-4	81
2	Squalene	410	C30H50	000111-02-4	72
3	Hexadeca-2,6,10,14-tetraen-1-ol,...	290	C20H34O	007614-21-3	64
4	4,8,12-Tetradecatrienal, 5,9,13-...	248	C17H28O	066408-55-7	64
5	Supraene	410	C30H50	007683-64-9	64





Tentatively Identified Compound (LSC) summary

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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Butane, 2-metho...	3.234	3.8	ng	36961	1	8.111	192475	20.0
Oxirane, [(1-me...	5.191	5.0	ng	48494	1	8.111	192475	20.0
Ethanol, 2-(2-b...	10.690	12.7	ng	171217	2	10.931	269172	20.0
n-Hexadecanoic ...	18.381	4.4	ng	119172	4	17.500	546333	20.0
Trifluoroacetox...	21.413	4.6	ng	148016	5	21.789	637786	20.0
Farnesol isomer a	23.540	2.7	ng	80163	6	25.114	592029	20.0