LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG101322\
Data File : BG055167.D
Acq On : 13 Oct 2022 17:15
Operator : CG/JU
Sample : N5105-09
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
WC-2

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-BG101322.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG055167.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.324	3	6	22	rVB	273212	433601	26.87%	4.146%
2	3.882	96	101	107	rBV	30884	47076	2.92%	0.450%
3	5.345	344	350	359	rVB	136859	210904	13.07%	2.017%
4	5.821	423	431	442	rBV	557878	886068	54.90%	8.472%
5	7.437	697	706	715	rBV	582464	1005004	62.27%	9.610%
6	8.300	847	853	864	rBV	148063	248300	15.39%	2.374%
7	9.475	1044	1053	1066	rBV	349674	624861	38.72%	5.975%
8	10.874	1285	1291	1304	rVB2	18677	33009	2.05%	0.316%
9	11.132	1327	1335	1343	rBV	212198	370055	22.93%	3.538%
10	13.541	1738	1745	1752	rVB	922920	1399712	86.73%	13.384%
11	14.346	1878	1882	1889	rVB	11939	18103	1.12%	0.173%
12	14.910	1966	1978	1986	rBV	331259	519366	32.18%	4.966%
13	16.385	2222	2229	2238	rBV	753778	1137503	70.48%	10.876%
14	17.642	2436	2443	2450	rBV	374490	565150	35.02%	5.404%
15	18.494	2584	2588	2601	rBV	46194	90615	5.61%	0.866%
16	20.216	2876	2881	2888	rBV	1256594	1613863	100.00%	15.431%
17	21.526	3100	3104	3111	rBV	78069	114960	7.12%	1.099%
18	21.925	3166	3172	3178	rVB	309811	550427	34.11%	5.263%
19	25.351	3746	3755	3768	rBV2	191220	589829	36.55%	5.640%

Sum of corrected areas: 10458406

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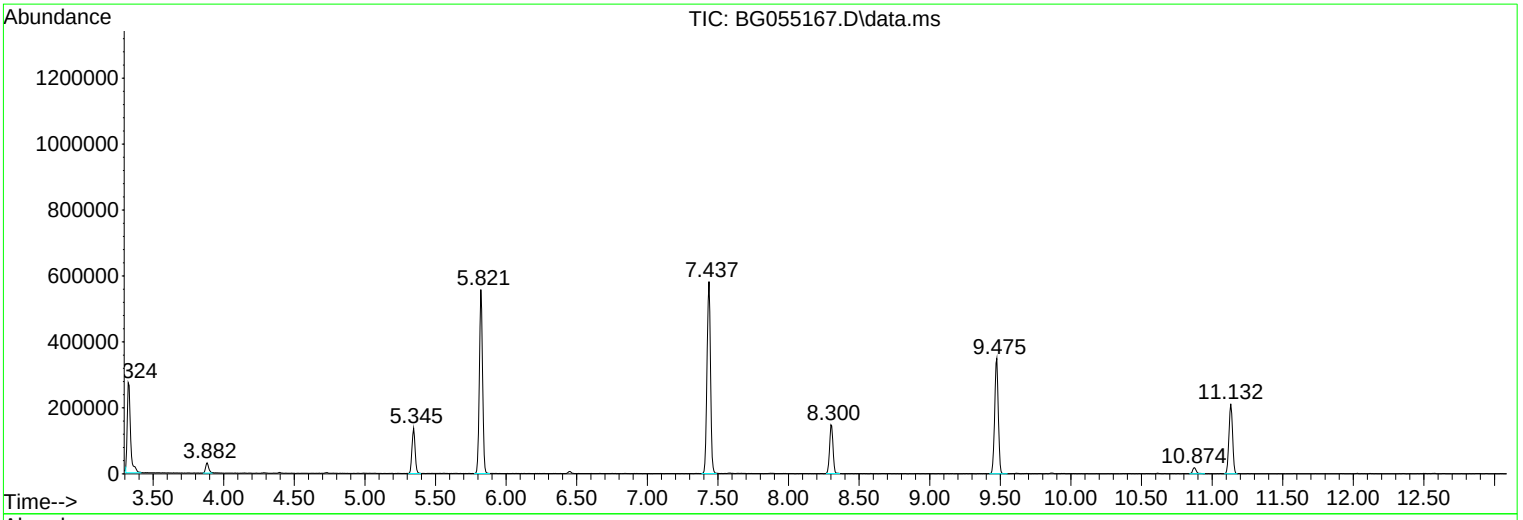
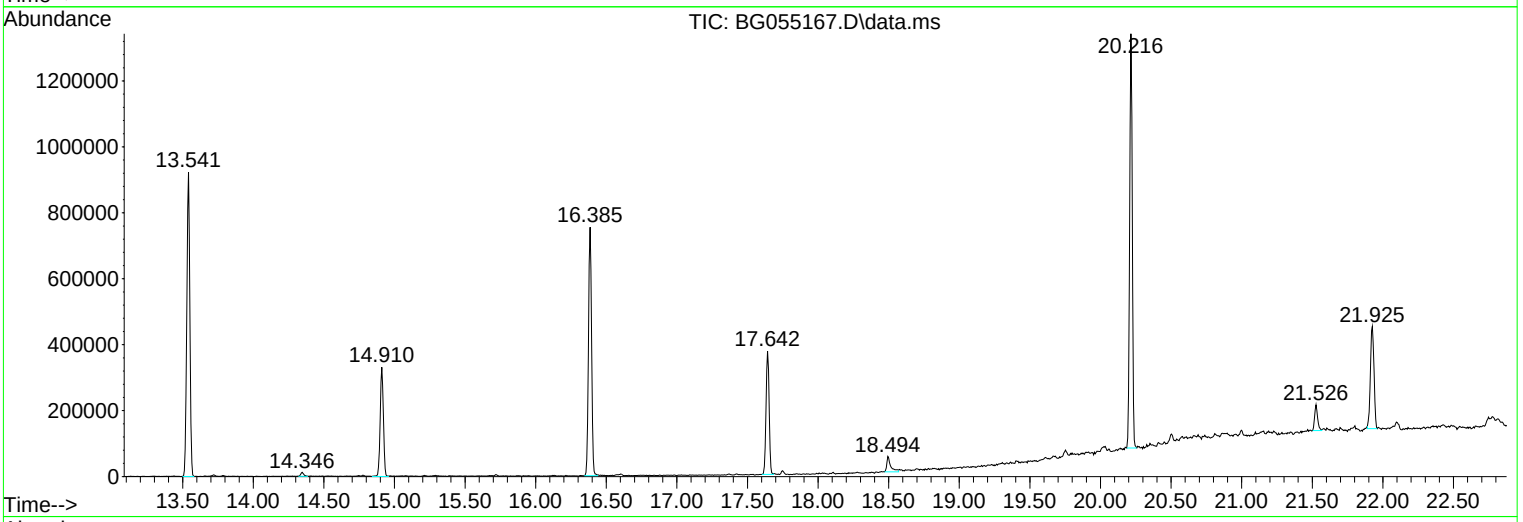
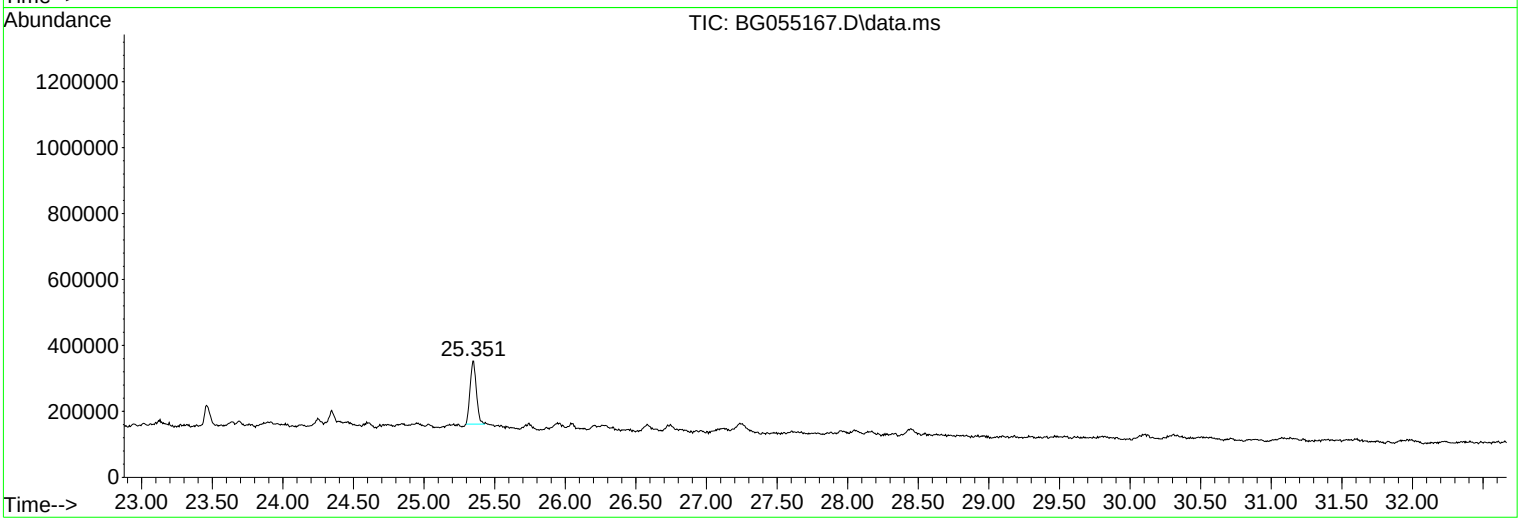
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG101322.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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







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TIC Library : C:\Database\NIST20.L
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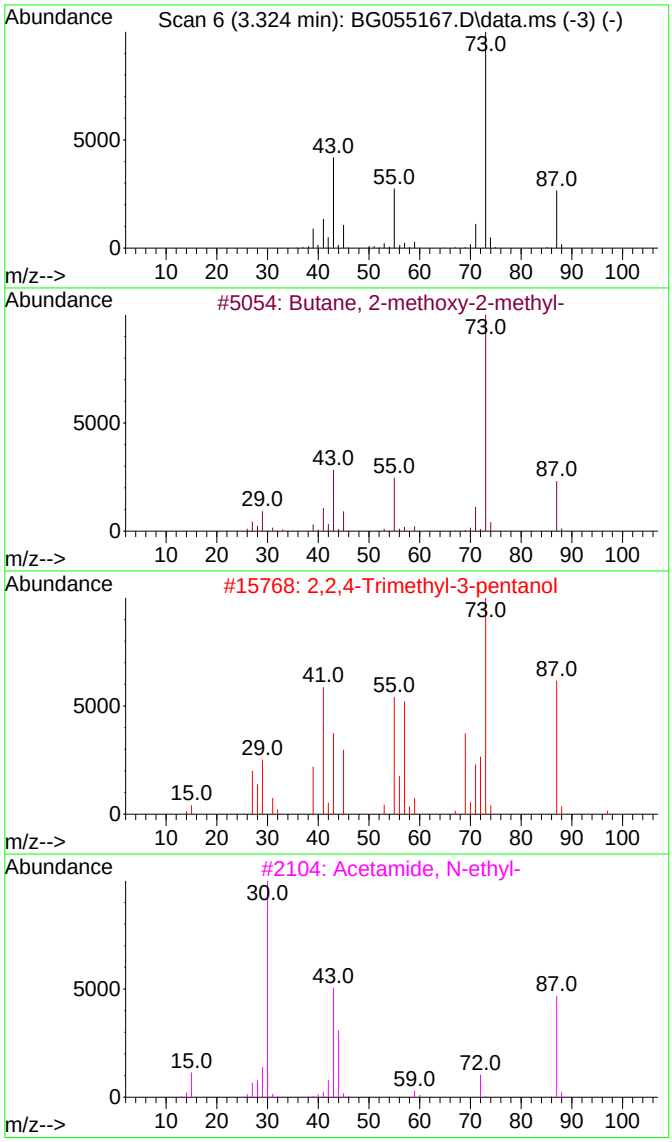
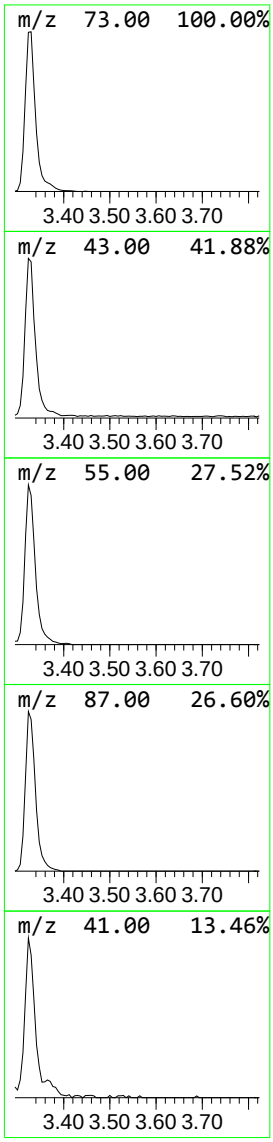
Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.324	34.93 ng	433601	1,4-Dichlorobenzene-d4	8.300

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	35
4	1,3-Dioxolane, 2-propyl-	116	C6H12O2	003390-13-4	17
5	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12





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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG101322.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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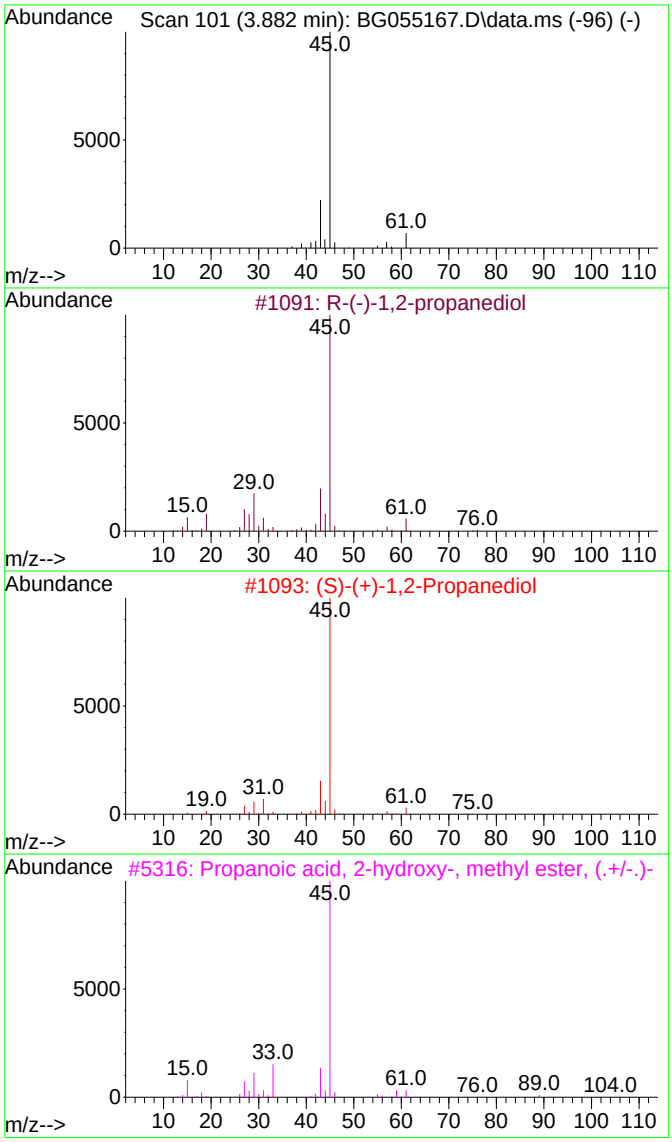
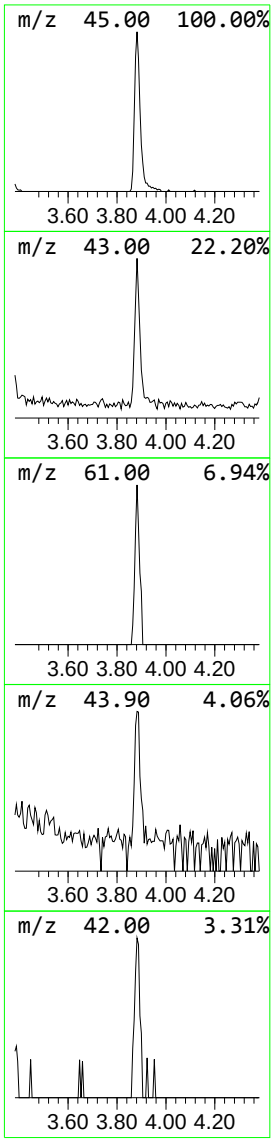
Peak Number 2 unknown3.882 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.882	3.79 ng	47076	1,4-Dichlorobenzene-d4	8.300

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	9
2	(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	9
3	Propanoic acid, 2-hydroxy-, meth...	104	C4H8O3	000547-64-8	9
4	Propylene Glycol	76	C3H8O2	000057-55-6	9
5	Formamide	45	CH3NO	000075-12-7	5





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Sample : N5105-09
Misc :
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Instrument :
BNA_G
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG101322.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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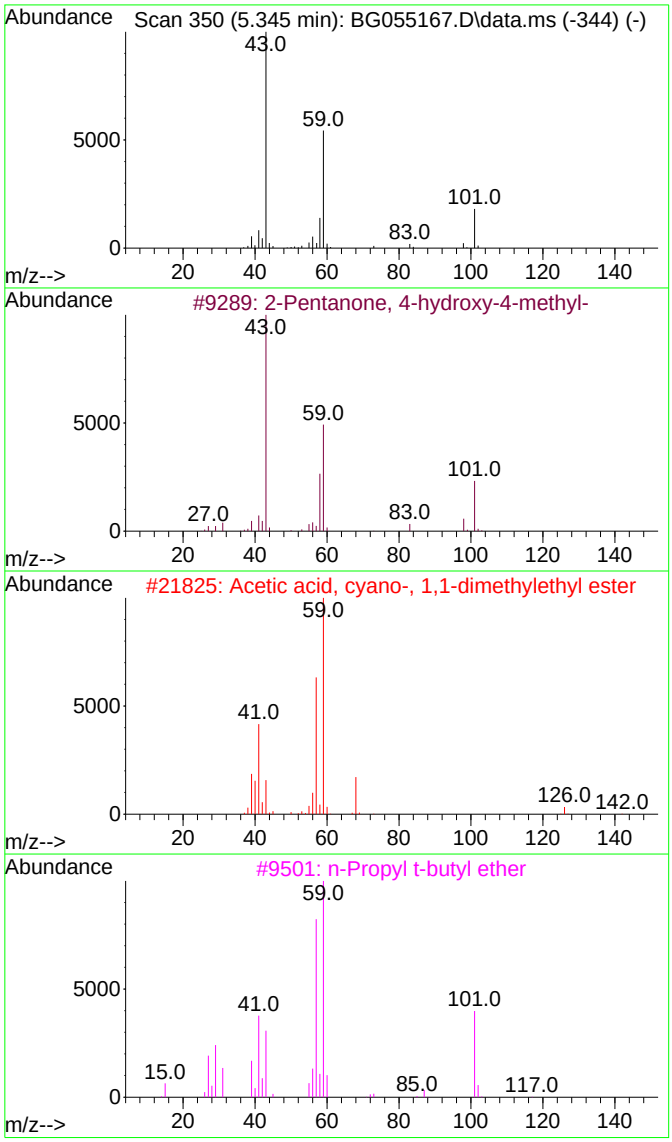
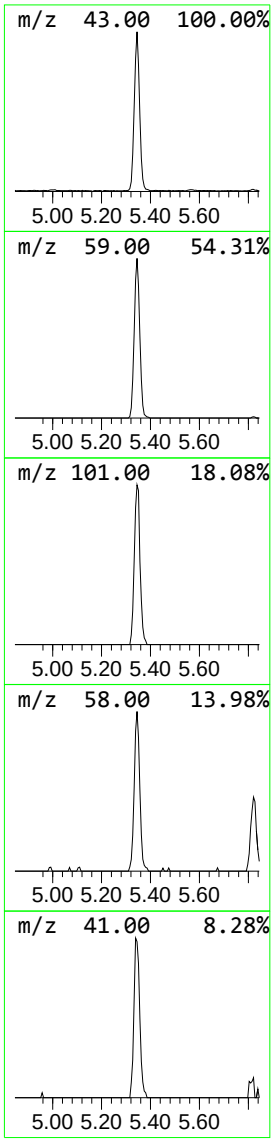
Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.345	16.99 ng	210904	1,4-Dichlorobenzene-d4	8.300

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	37
3	n-Propyl t-butyl ether	116	C7H16O	1000334-81-9	33
4	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
5	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28





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TIC Library : C:\Database\NIST20.L
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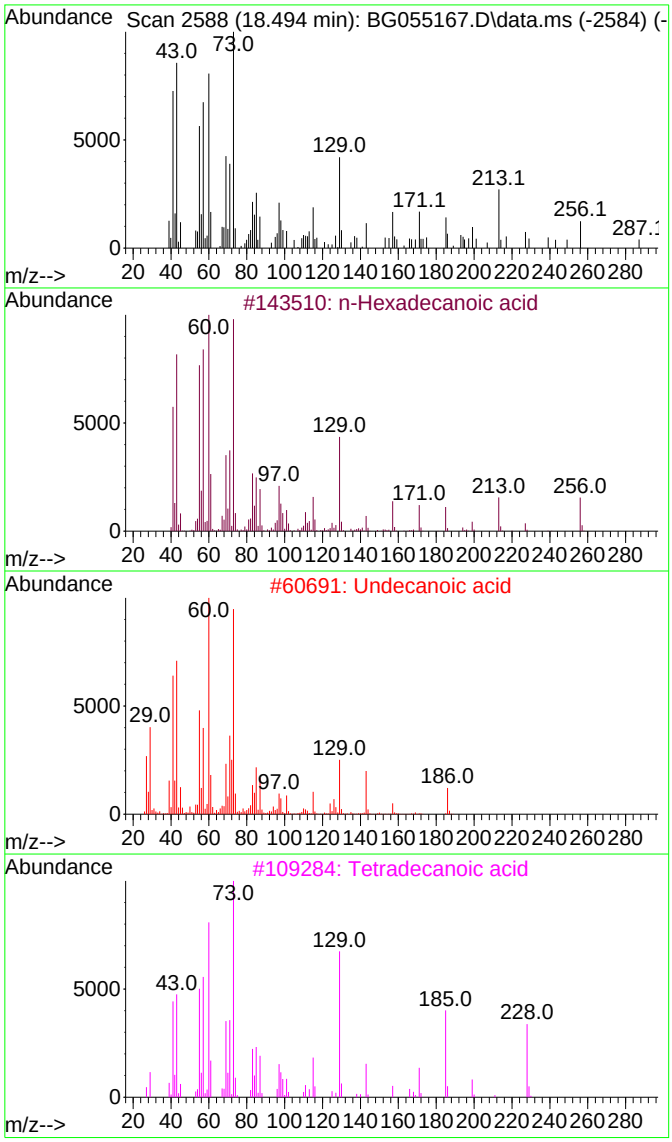
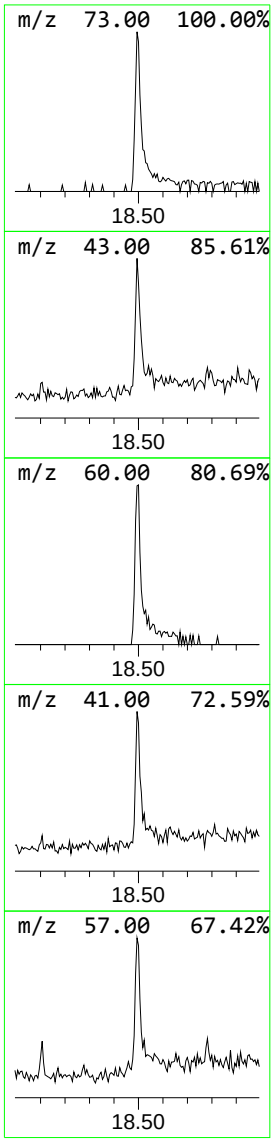
Peak Number 4 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.494	3.21 ng	90615	Phenanthrene-d10	17.642

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Undecanoic acid	186	C11H22O2	000112-37-8	72
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	72
4	Tridecanoic acid	214	C13H26O2	000638-53-9	70
5	n-Decanoic acid	172	C10H20O2	000334-48-5	70





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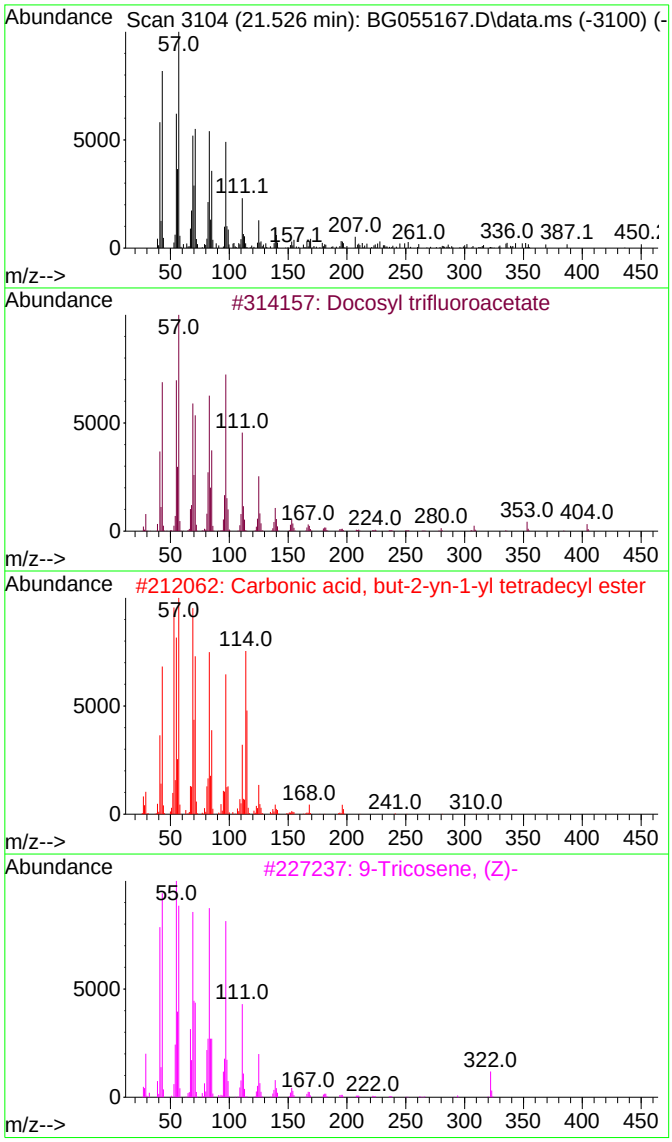
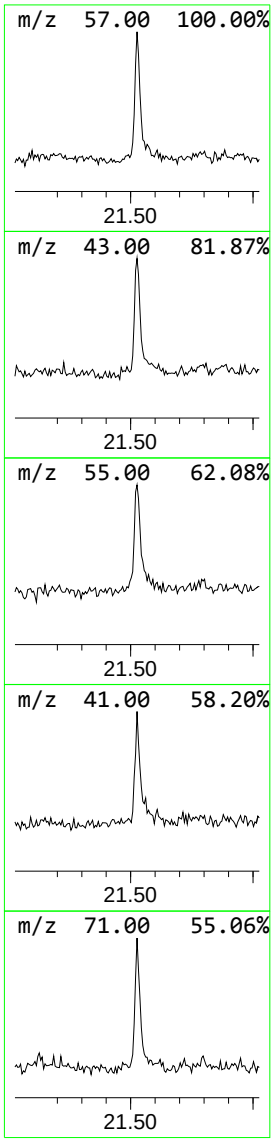
Peak Number 5 Docosyl trifluoroacetate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.526	4.18 ng	114960	Chrysene-d12	21.926

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Docosyl trifluoroacetate	422	C24H45F3O2	1000351-75-5	91
2	Carbonic acid, but-2-yn-1-yl tet...	310	C19H34O3	1010383-20-9	91
3	9-Tricosene, (Z)-	322	C23H46	027519-02-4	90
4	1-Octadecene	252	C18H36	000112-88-9	90
5	1-Tetracosene	336	C24H48	010192-32-2	89





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...	3.324	34.9	ng	433601	1	8.300	248300	20.0
unknown3.882	3.882	3.8	ng	47076	1	8.300	248300	20.0
2-Pentanone, 4-...	5.345	17.0	ng	210904	1	8.300	248300	20.0
n-Hexadecanoic ...	18.494	3.2	ng	90615	4	17.642	565150	20.0
Docosyl trifluo...	21.526	4.2	ng	114960	5	21.926	550427	20.0