LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062823\
Data File : BG057889.D
Acq On : 28 Jun 2023 12:28
Operator : CG/JU
Sample : 03368-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
CF-28

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-BG062723.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG057889.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.023	322	329	335	rBV2	35331	53758	2.33%	0.348%
2	5.493	402	409	420	rBV	880751	1390064	60.14%	8.995%
3	7.085	671	680	691	rBV	870488	1508435	65.26%	9.761%
4	7.919	815	822	829	rBV	216891	369843	16.00%	2.393%
5	9.077	1011	1019	1028	rBV	515108	912768	39.49%	5.907%
6	10.722	1289	1299	1306	rBV	325492	562693	24.34%	3.641%
7	13.178	1710	1717	1725	rVB	1253669	1889864	81.76%	12.230%
8	13.877	1832	1836	1842	rVB3	19273	28367	1.23%	0.184%
9	14.265	1897	1902	1913	rBV	54134	82769	3.58%	0.536%
10	14.553	1945	1951	1959	rVB	479743	746644	32.30%	4.832%
11	15.910	2176	2182	2188	rBV	202571	285085	12.33%	1.845%
12	16.039	2197	2204	2214	rBV	996922	1518113	65.68%	9.824%
13	17.297	2410	2418	2424	rBV	562534	868545	37.58%	5.621%
14	17.485	2443	2450	2456	rBV4	28801	52964	2.29%	0.343%
15	18.184	2565	2569	2581	rBV	156531	316734	13.70%	2.050%
16	18.918	2691	2694	2699	rVB5	20980	28871	1.25%	0.187%
17	19.353	2764	2768	2773	rBV	53344	76652	3.32%	0.496%
18	19.406	2773	2777	2782	rVB	61249	79740	3.45%	0.516%
19	19.465	2783	2787	2797	rBV7	39941	91779	3.97%	0.594%
20	19.717	2826	2830	2835	rVB	51193	72613	3.14%	0.470%
21	19.917	2858	2864	2869	rBV	1761582	2311398	100.00%	14.958%
22	21.204	3079	3083	3094	rBV	241656	441414	19.10%	2.856%
23	21.556	3137	3143	3148	rBV	510049	853011	36.90%	5.520%
24	24.711	3673	3680	3692	rBV	308256	910959	39.41%	5.895%

Sum of corrected areas: 15453083

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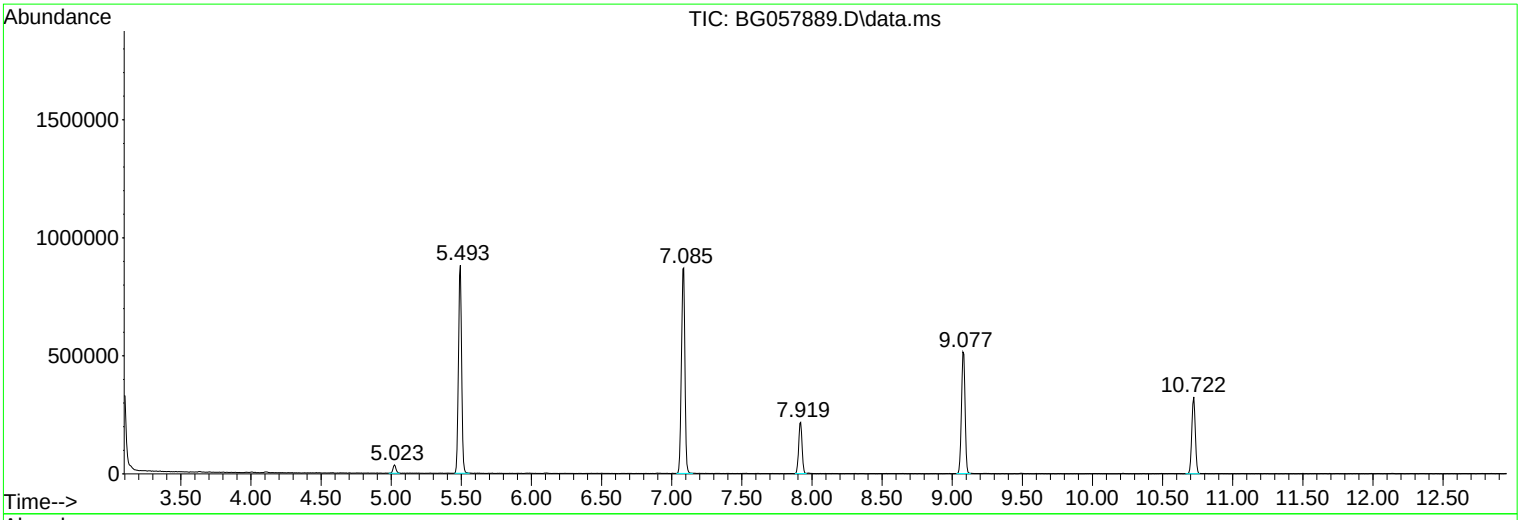
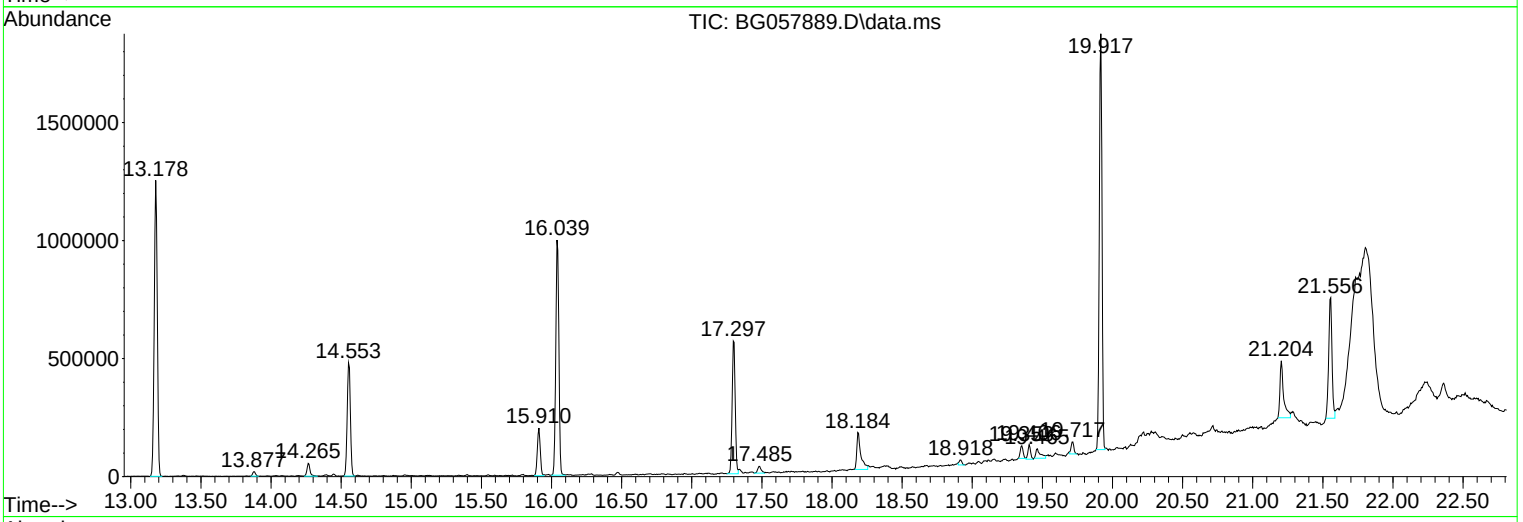
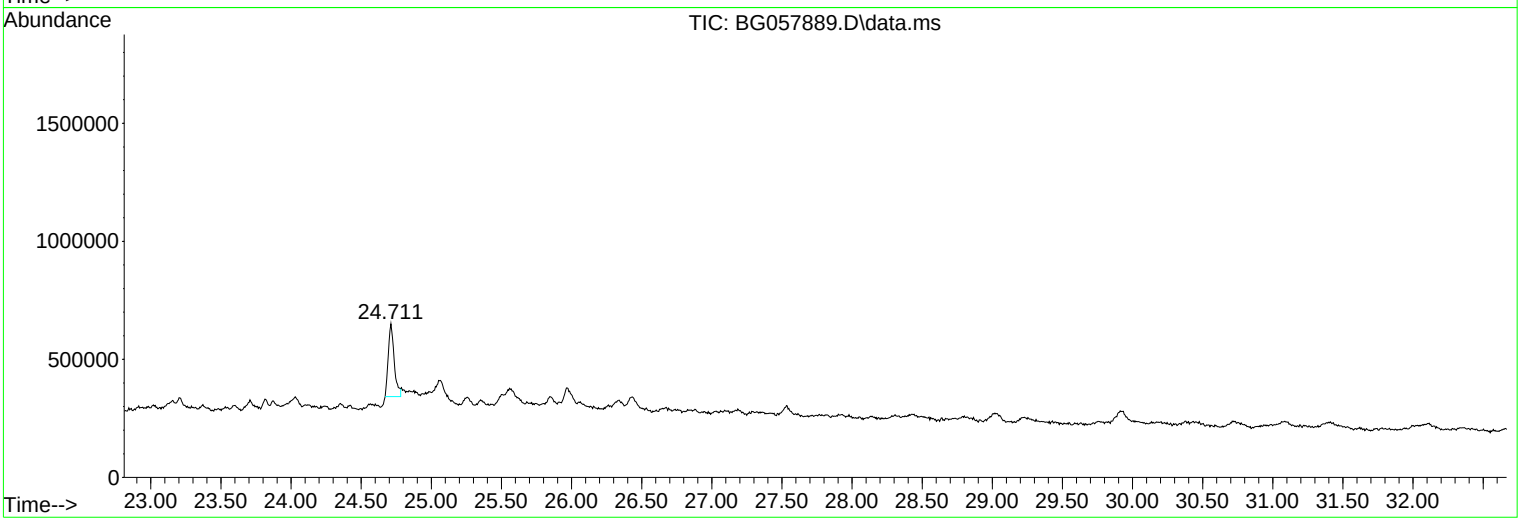
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG062723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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







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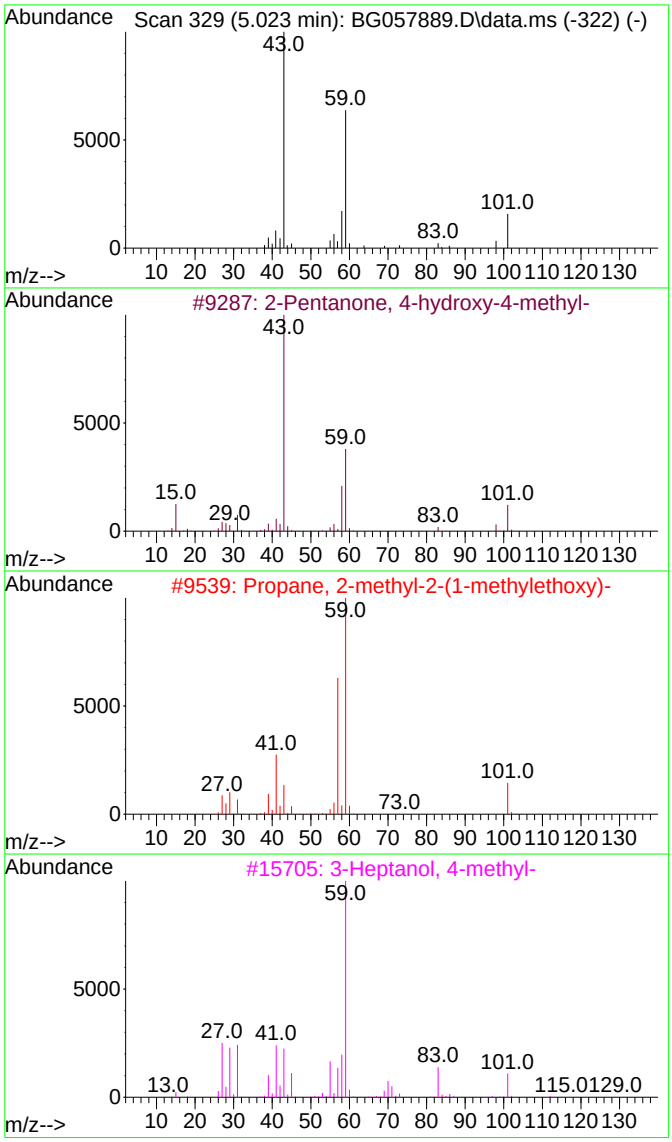
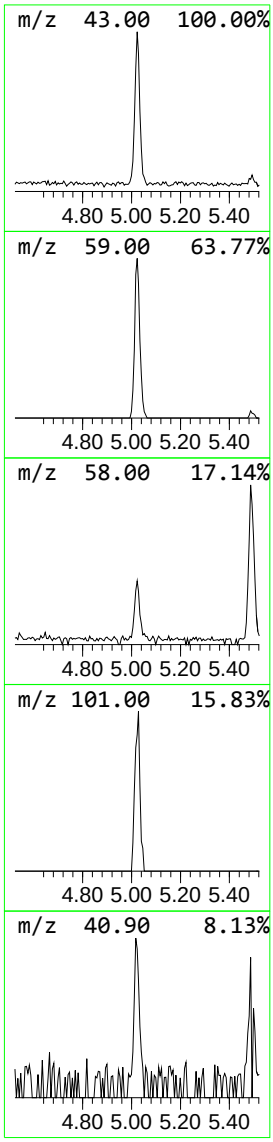
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.023	2.91 ng	53758	1,4-Dichlorobenzene-d4	7.919

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	33
3	3-Heptanol, 4-methyl-	130	C8H18O	014979-39-6	33
4	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
5	Pentanal, oxime	101	C5H11NO	000628-79-5	28





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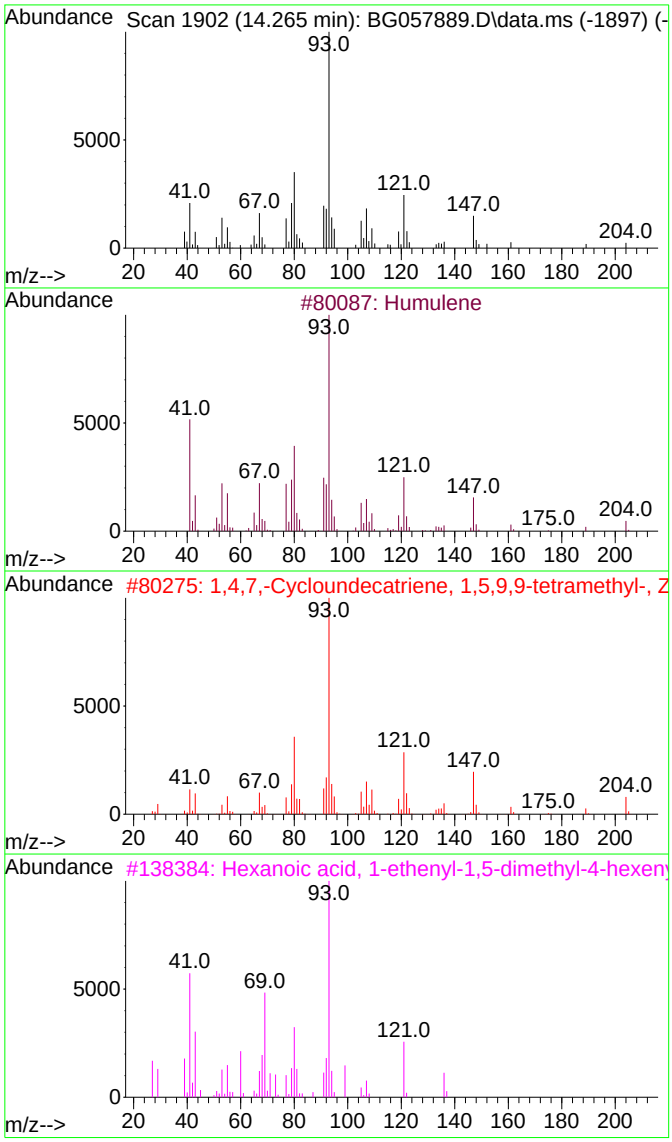
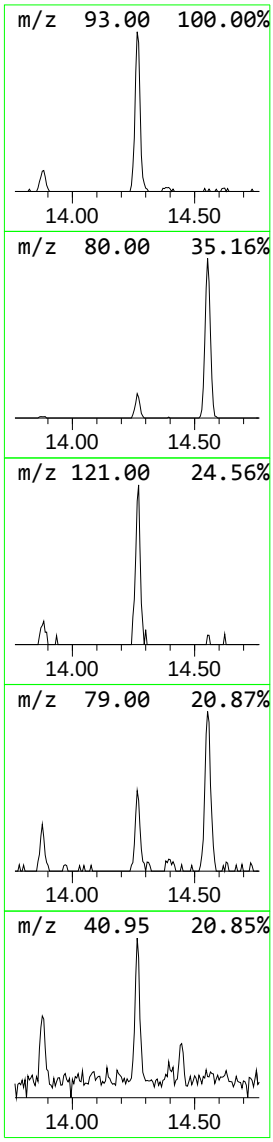
****

Peak Number 2 Humulene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.265	2.22 ng	82769	Acenaphthene-d10	14.553

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Humulene	204	C15H24	006753-98-6	97
2	1,4,7,-Cycloundecatriene, 1,5,9,...	204	C15H24	1000062-61-9	95
3	Hexanoic acid, 1-ethenyl-1,5-dim...	252	C16H28O2	007779-23-9	59
4	Tricyclo[2.2.1.0(2,6)]heptane, 1...	136	C10H16	000488-97-1	59
5	1,5-Dimethyl-1-vinyl-4-hexenyl b...	224	C14H24O2	000078-36-4	53





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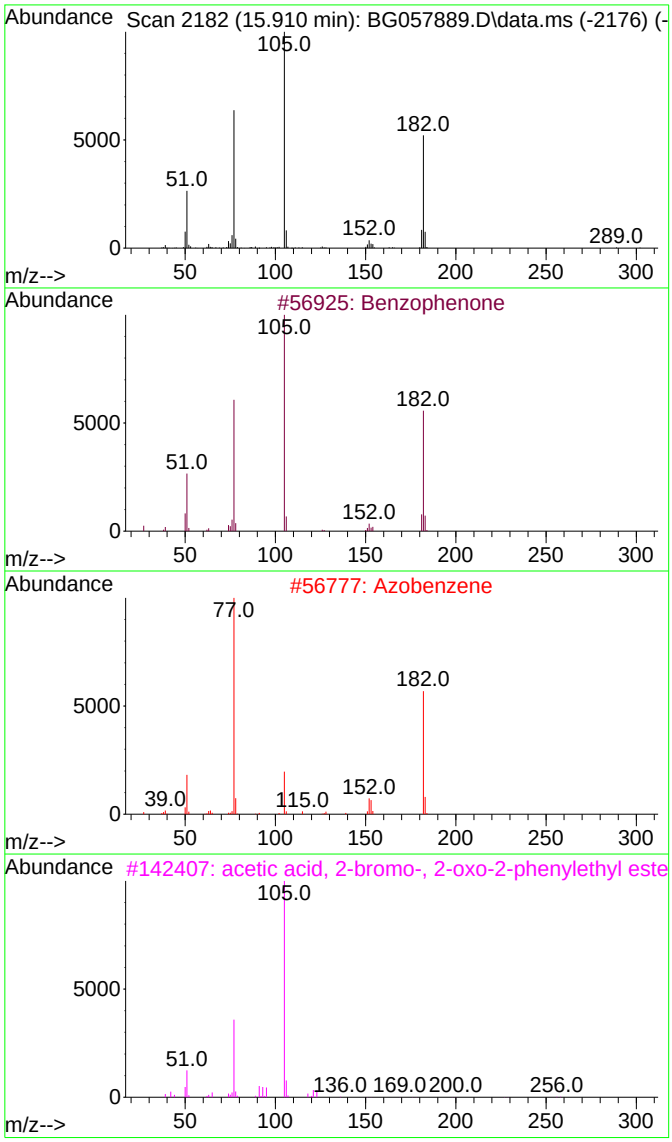
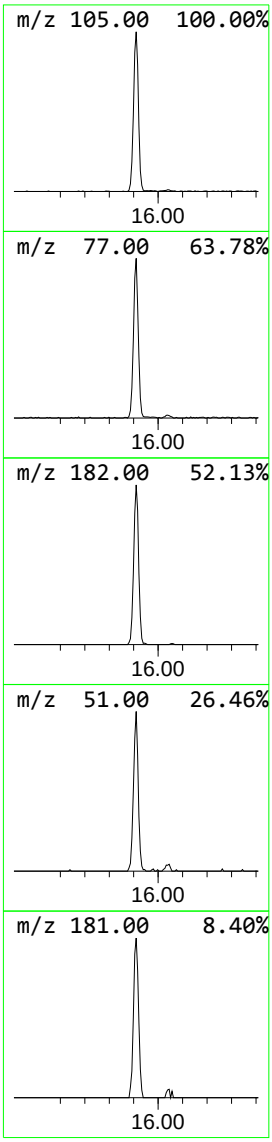
****

Peak Number 3 Benzophenone Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.910	7.64 ng	285085	Acenaphthene-d10	14.553

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	96
2	Azobenzene	182	C12H10N2	000103-33-3	59
3	acetic acid, 2-bromo-, 2-oxo-2-p...	256	C10H9BrO3	1000401-50-0	47
4	Disulfide, dibenzoyl	274	C14H10O2S2	000644-32-6	47
5	N-cyanobenzamide	146	C8H6N2O	015150-25-1	47





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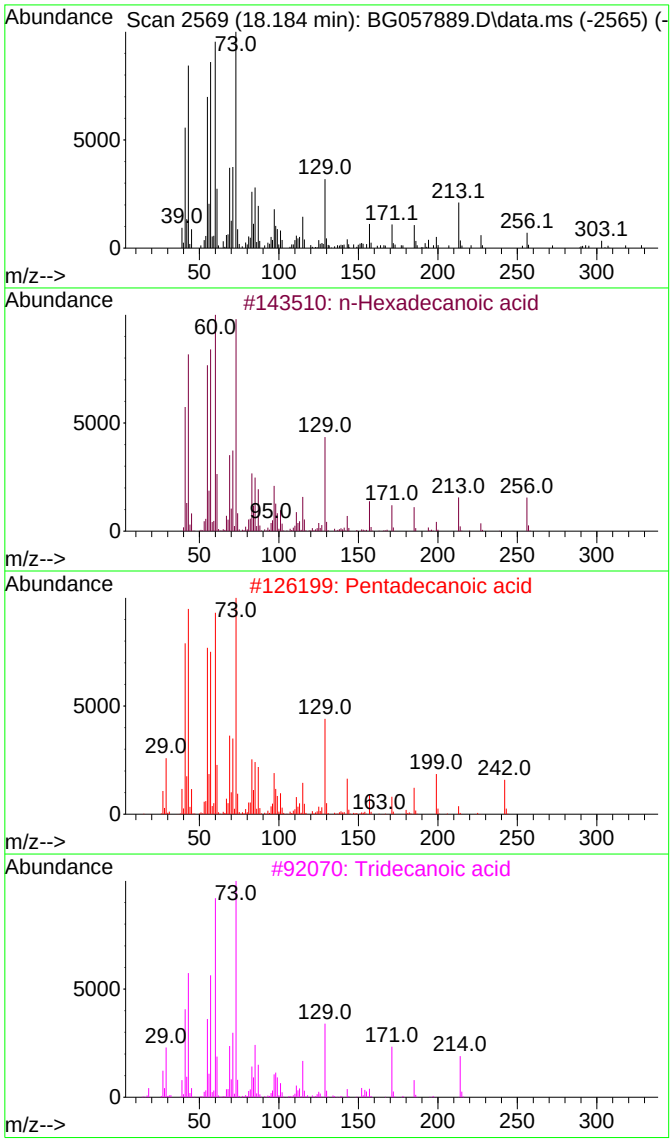
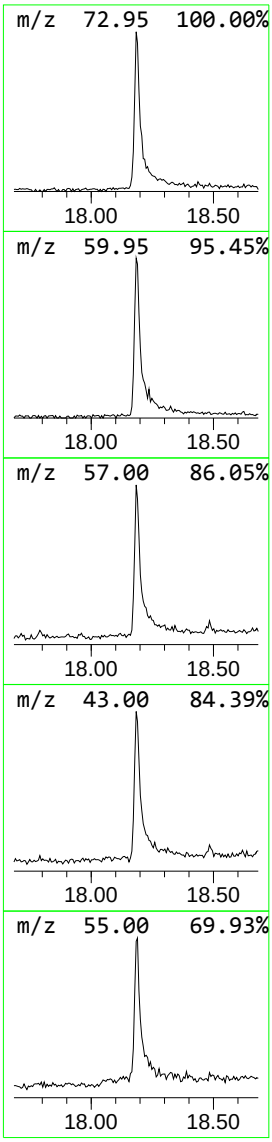
Peak Number 4 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.184	7.29 ng	316734	Phenanthrene-d10	17.302

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	87
3	Tridecanoic acid	214	C13H26O2	000638-53-9	81
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	80
5	Octanoic acid	144	C8H16O2	000124-07-2	62





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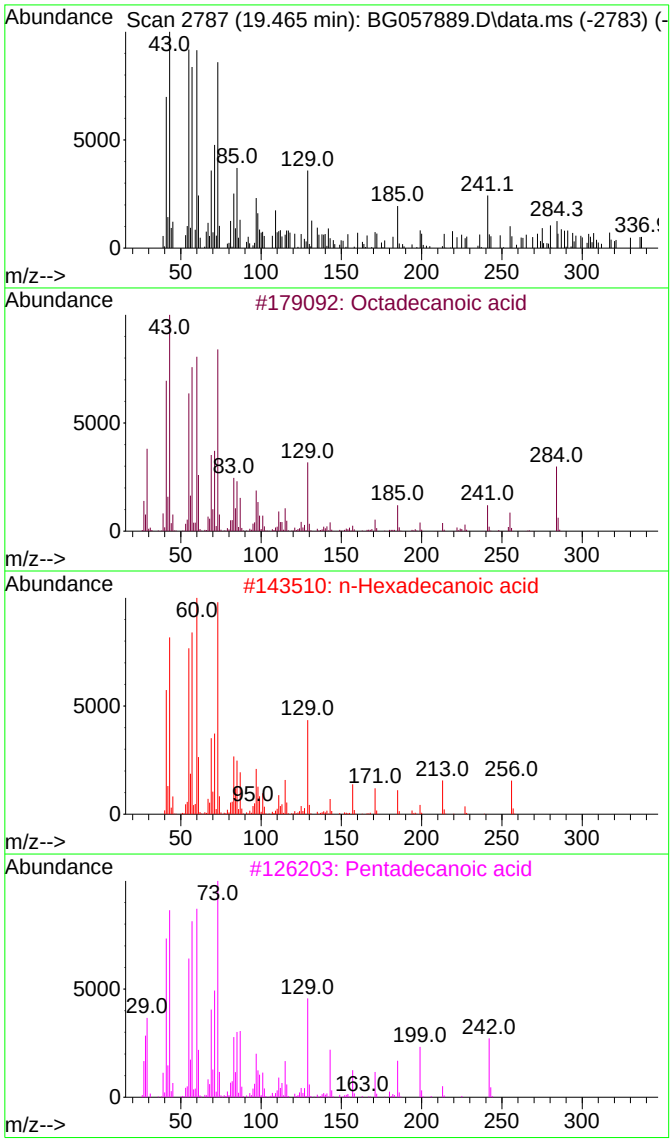
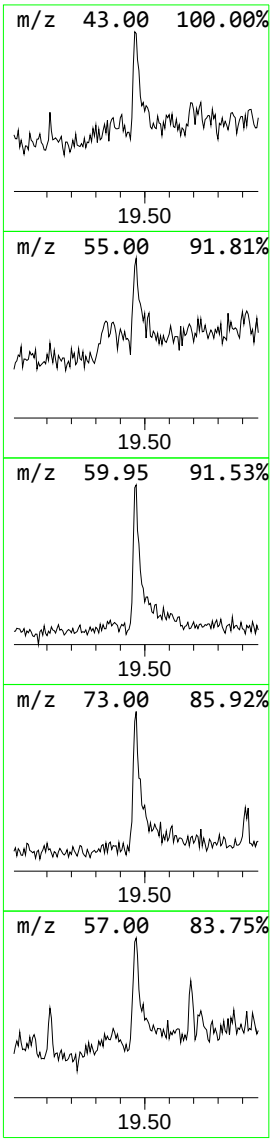
****

Peak Number 5 Octadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.465	2.15 ng	91779	Chrysene-d12	21.556

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	96
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	86
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	83
4	n-Decanoic acid	172	C10H20O2	000334-48-5	49
5	Tridecanoic acid	214	C13H26O2	000638-53-9	47





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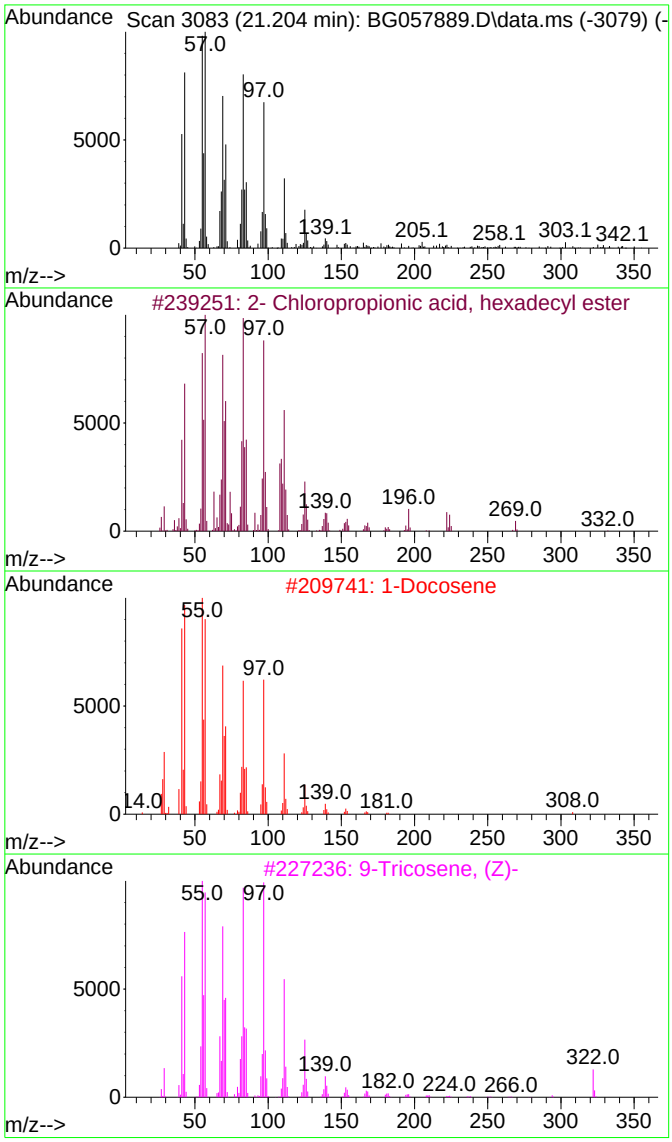
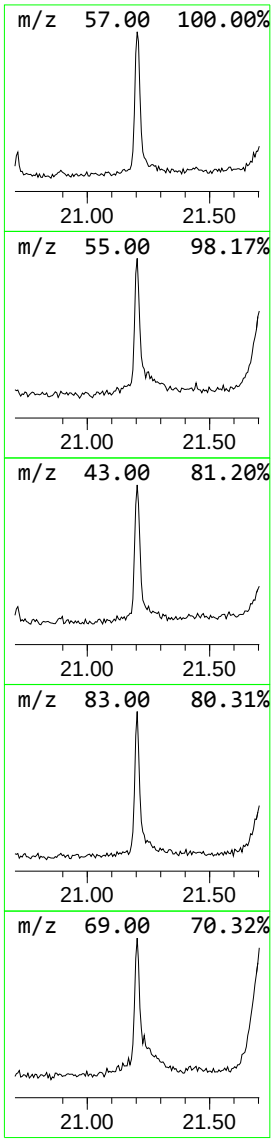
****
Peak Number 6 2- Chloropropionic acid, he... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.204	10.35 ng	441414	Chrysene-d12	21.556

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2- Chloropropionic acid, hexadec...	332	C19H37ClO2	086711-81-1	96
2	1-Docosene	308	C22H44	001599-67-3	94
3	9-Tricosene, (Z)-	322	C23H46	027519-02-4	94
4	Heptafluorobutyric acid, n-tetra...	410	C18H29F7O2	007365-36-8	94
5	2- Bromopropionic acid, tetradec...	348	C17H33BrO2	086711-82-2	91





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
2-Pentanone, 4-...	5.023	2.9	ng	53758	1	7.919	369843	20.0
Humulene	14.265	2.2	ng	82769	3	14.553	746644	20.0
Benzophenone	15.910	7.6	ng	285085	3	14.553	746644	20.0
n-Hexadecanoic ...	18.184	7.3	ng	316734	4	17.302	868545	20.0
Octadecanoic acid	19.465	2.1	ng	91779	5	21.556	853011	20.0
2- Chloropropio...	21.204	10.4	ng	441414	5	21.556	853011	20.0