LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG052223\
Data File : BG057492.D
Acq On : 22 May 2023 13:49
Operator : CG/JU
Sample : 02849-41
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TP11

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-BG042723.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG057492.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.384	309	314	324	rVB	16669	25135	2.10%	0.448%
2	5.878	391	398	409	rBB	249838	405486	33.93%	7.223%
3	7.499	667	674	685	rBV	259170	457205	38.26%	8.144%
4	8.357	814	820	827	rBB	71635	116986	9.79%	2.084%
5	9.537	1011	1021	1031	rBV	157941	285199	23.86%	5.080%
6	11.194	1296	1303	1313	rVB	93994	160846	13.46%	2.865%
7	13.597	1705	1712	1721	rBV	462033	711673	59.55%	12.677%
8	14.913	1931	1936	1941	rBV	32134	43834	3.67%	0.781%
9	14.971	1941	1946	1957	rVB	154751	247653	20.72%	4.411%
10	16.311	2168	2174	2181	rVB	26972	40077	3.35%	0.714%
11	16.458	2193	2199	2206	rVB	390410	603656	50.51%	10.753%
12	17.715	2407	2413	2421	rBV	223632	338711	28.34%	6.033%
13	20.282	2844	2850	2860	rBV	935107	1195127	100.00%	21.289%
14	21.233	3008	3012	3016	rBV6	7849	12030	1.01%	0.214%
15	21.416	3038	3043	3048	rVB	142484	192826	16.13%	3.435%
16	21.580	3066	3071	3081	rBV5	22686	53921	4.51%	0.960%
17	22.021	3139	3146	3154	rBV	207989	362953	30.37%	6.465%
18	24.411	3549	3553	3559	rVB5	15031	25795	2.16%	0.459%
19	25.528	3733	3743	3753	rBV	110757	334839	28.02%	5.964%

Sum of corrected areas: 5613952

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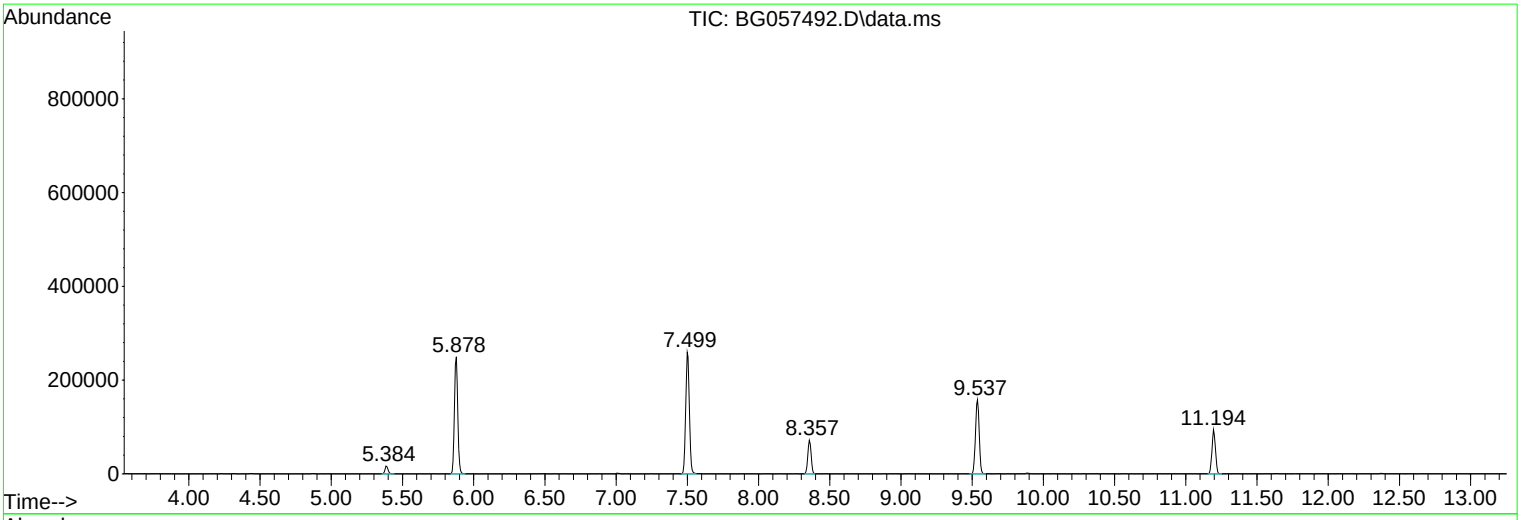
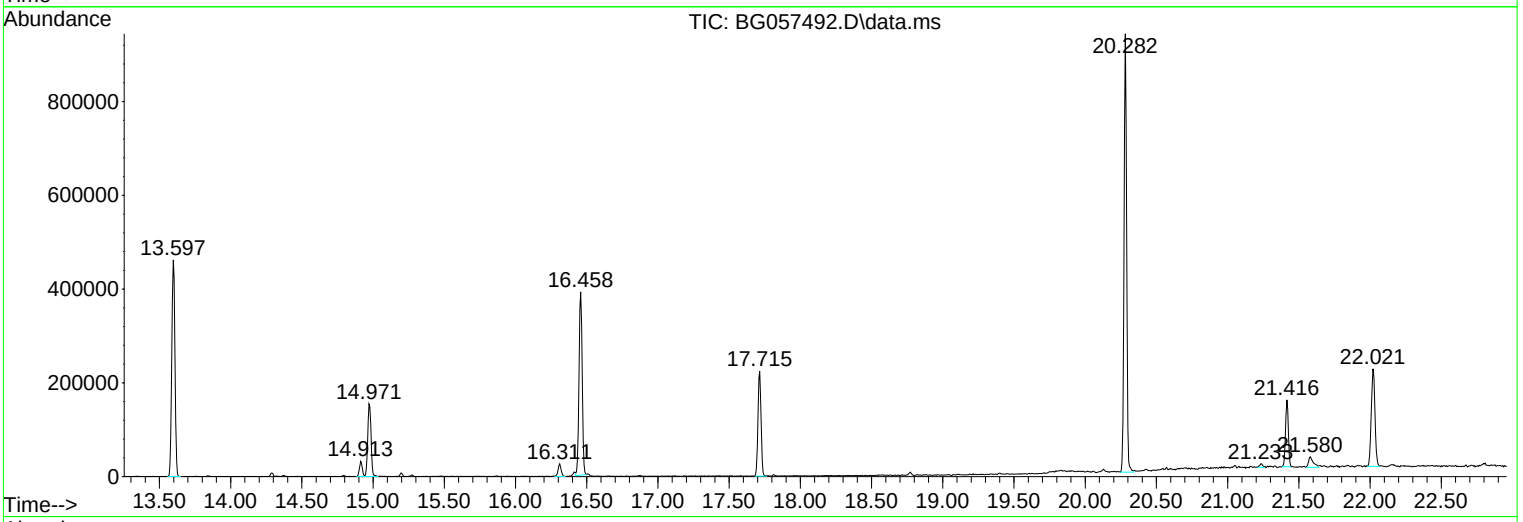
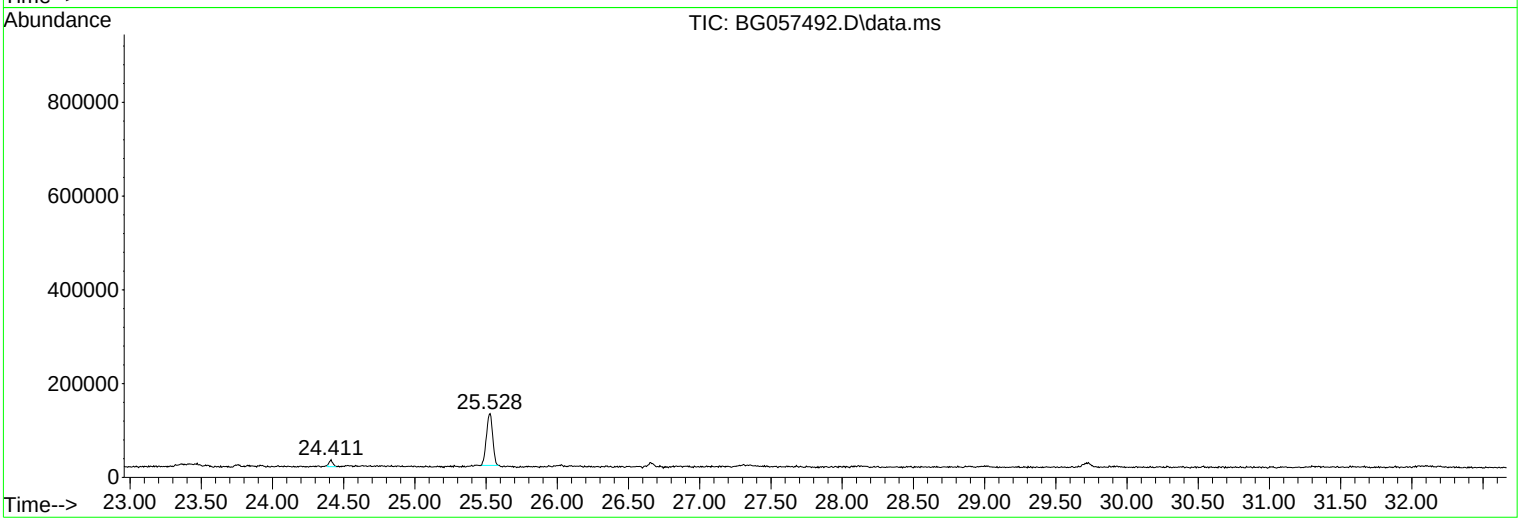
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG042723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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







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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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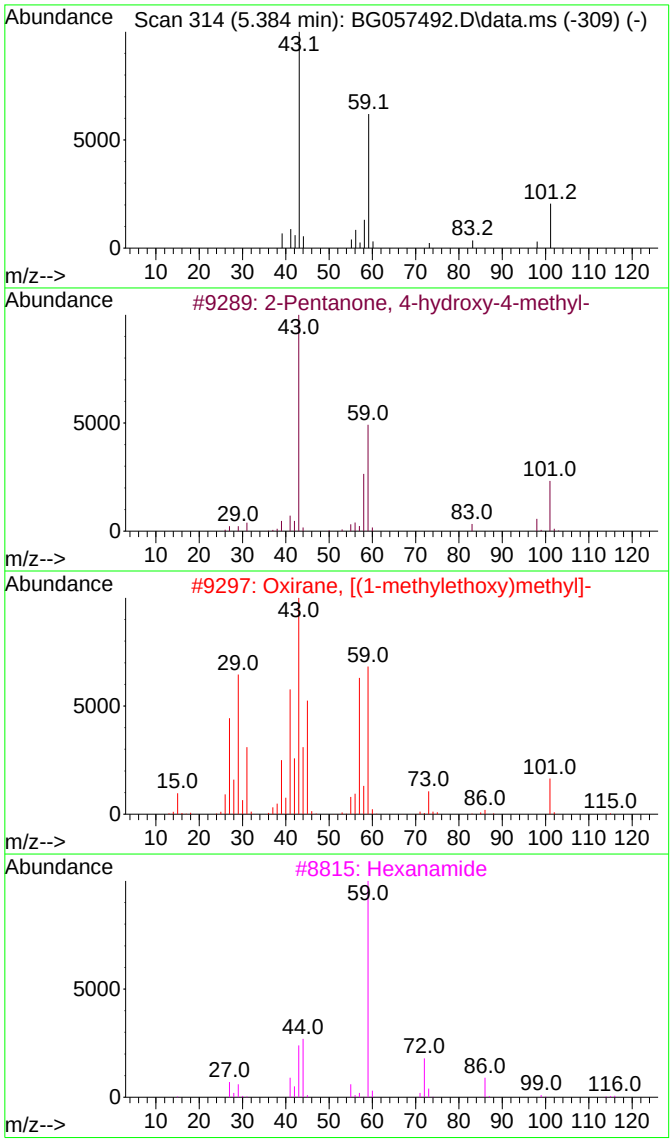
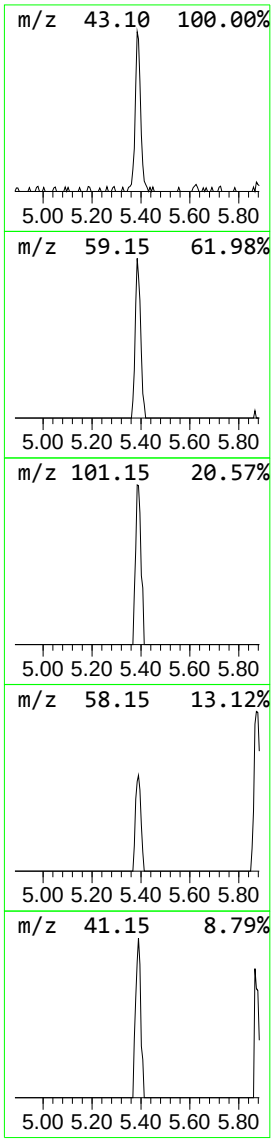
****
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.384	4.30 ng	25135	1,4-Dichlorobenzene-d4	8.357

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	Oxirane, [(1-methylethoxy)methyl]-	116	C6H12O2	004016-14-2	38
3	Hexanamide	115	C6H13NO	000628-02-4	17
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	9





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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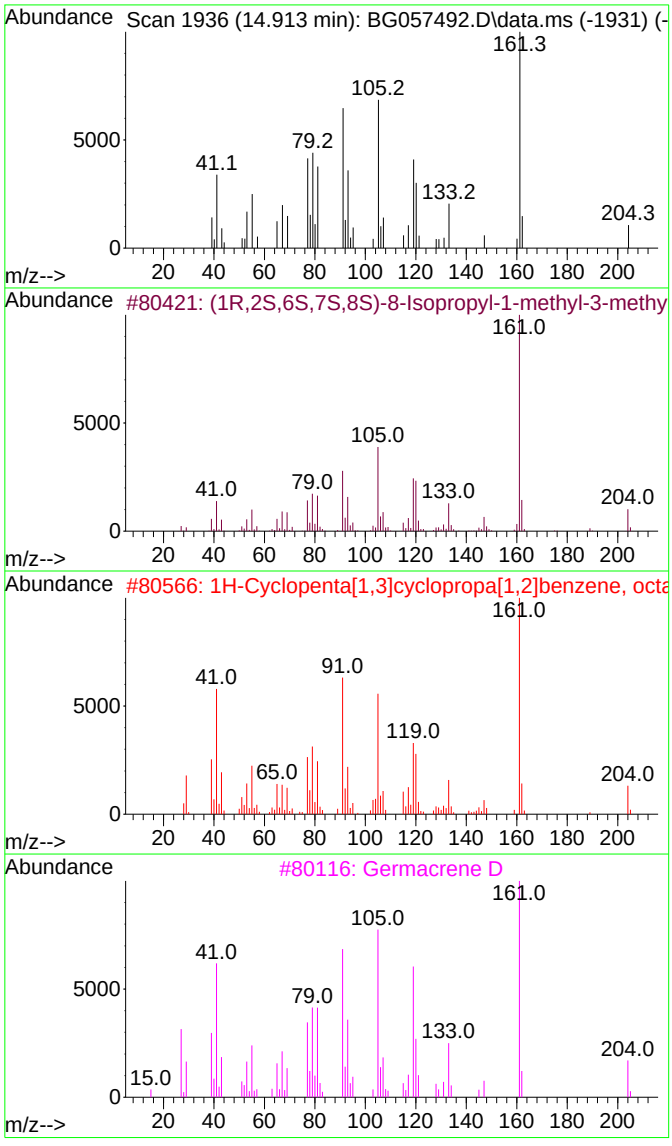
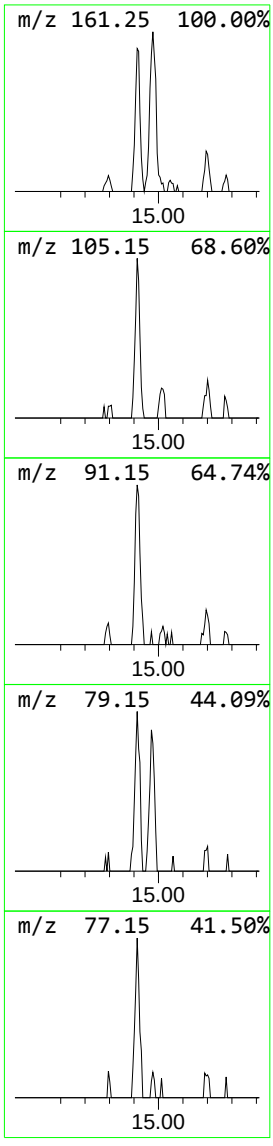
****
Peak Number 2 (1R,2S,6S,7S,8S)-8-Isopropy... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.913	3.54 ng	43834	Acenaphthene-d10	14.971

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(1R,2S,6S,7S,8S)-8-Isopropyl-1-m...	204	C15H24	018252-44-3	98
2	1H-Cyclopenta[1,3]cyclopropa[1,2...	204	C15H24	013744-15-5	95
3	Germacrene D	204	C15H24	023986-74-5	91
4	cis-Muurola-4(15),5-diene	204	C15H24	157477-72-0	55
5	2-(3-Methyl-but-1-ynyl)-cyclohex...	176	C12H16O	106180-26-1	53





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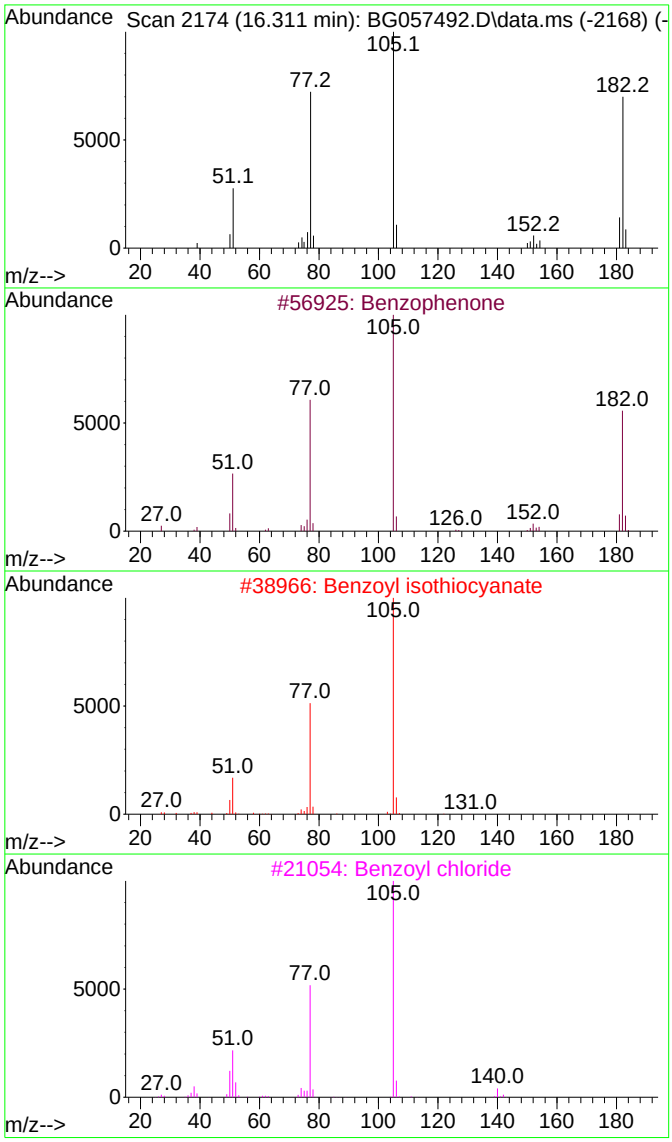
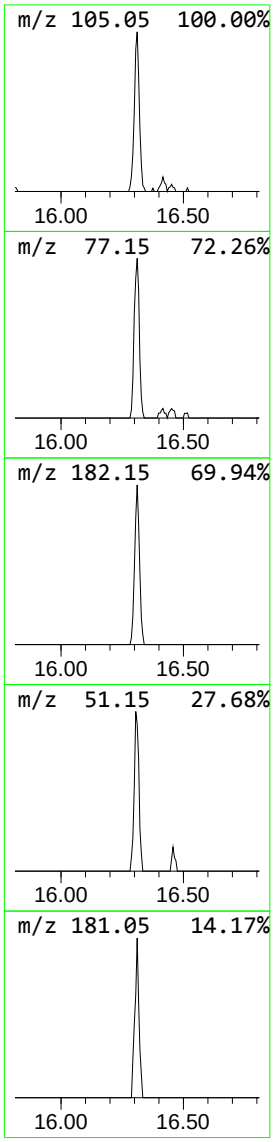
Peak Number 3 Benzophenone Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.311	3.24 ng	40077	Acenaphthene-d10	14.971

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	97
2	Benzoyl isothiocyanate	163	C8H5NOS	000532-55-8	47
3	Benzoyl chloride	140	C7H5ClO	000098-88-4	47
4	Acetophenone, 2-chloro-	154	C8H7ClO	000532-27-4	47
5	N-cyanobenzamide	146	C8H6N2O	015150-25-1	47





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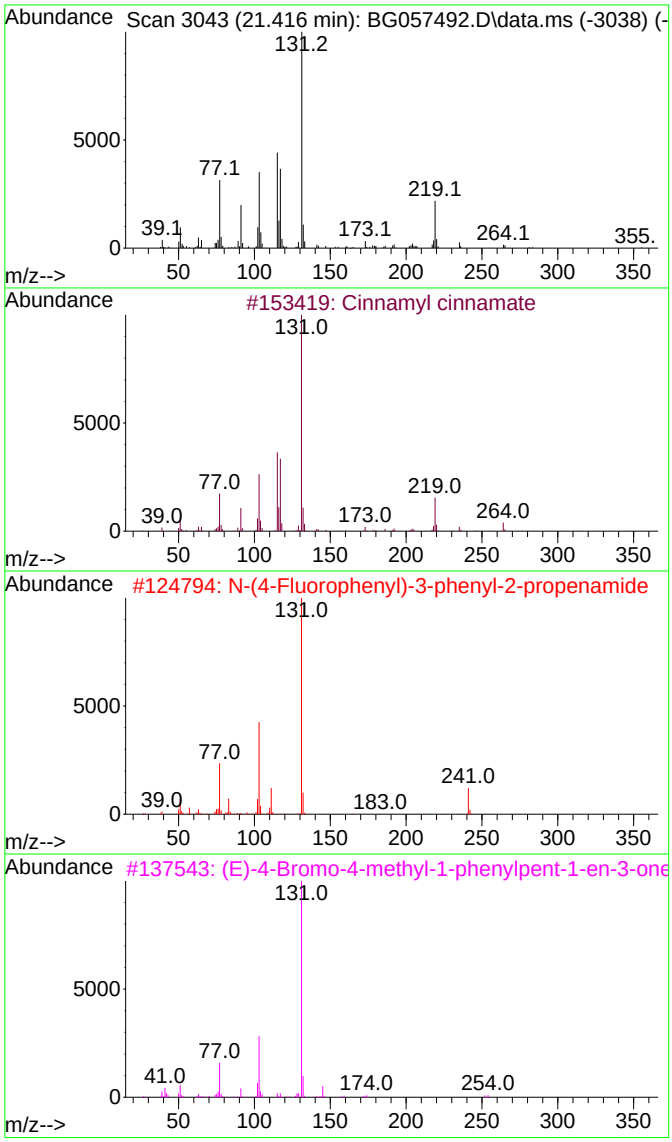
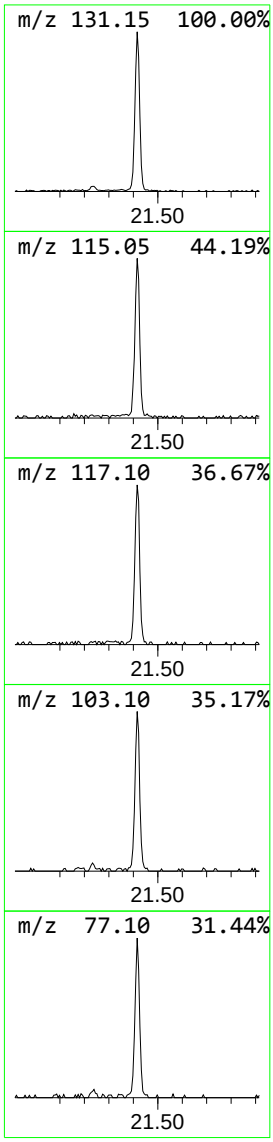
Peak Number 4 Cinnamyl cinnamate Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.416	10.63 ng	192826	Chrysene-d12	22.021

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cinnamyl cinnamate	264	C18H16O2	000122-69-0	91
2	N-(4-Fluorophenyl)-3-phenyl-2-pr...	241	C15H12FNO	019358-27-1	47
3	(E)-4-Bromo-4-methyl-1-phenylpen...	252	C12H13BrO	1000443-02-8	47
4	1-Penten-3-one, 4,4-dimethyl-1-p...	188	C13H16O	000538-44-3	47
5	2,2-Dimethyl-1-(2-vinylphenyl)pr...	188	C13H16O	1000210-99-9	47





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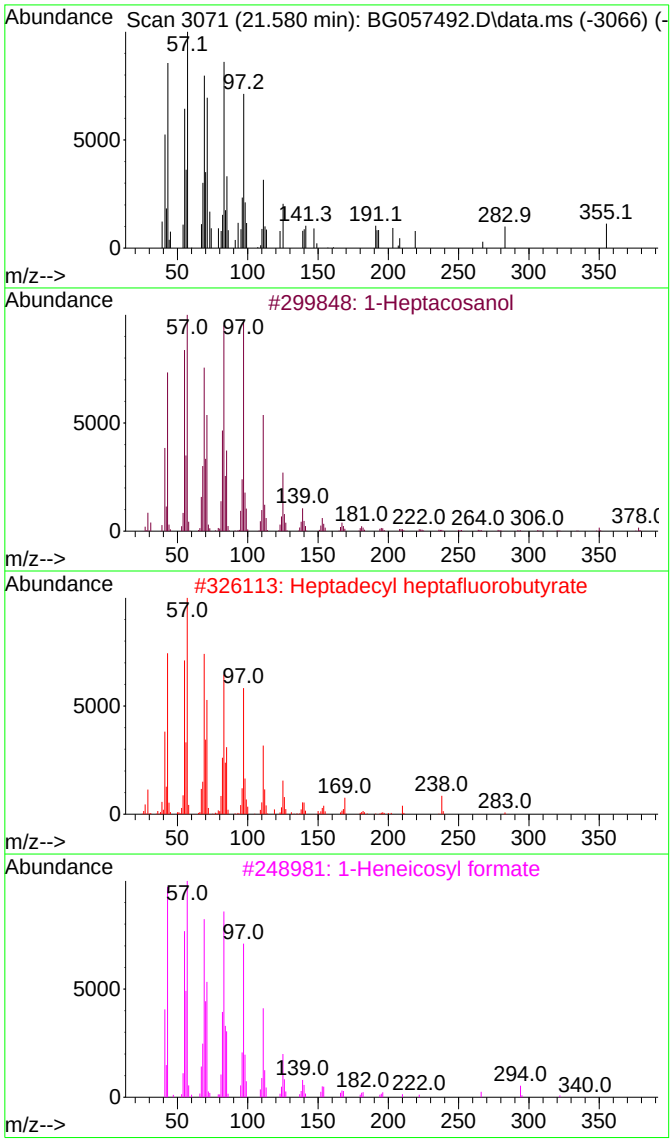
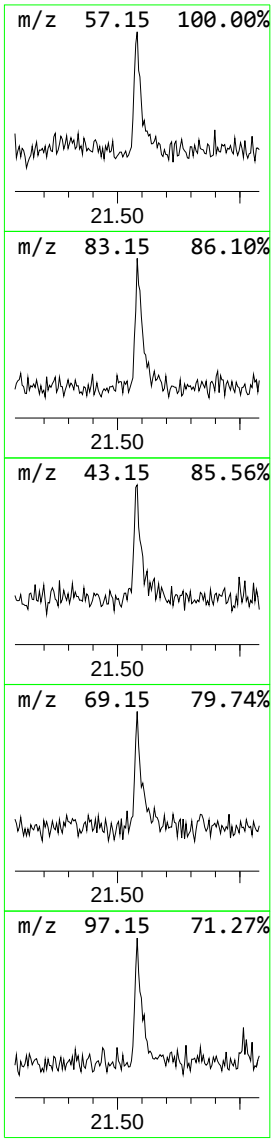
****

Peak Number 5 1-Heptacosanol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.580	2.97 ng	53921	Chrysene-d12	22.021

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heptacosanol	396	C27H56O	002004-39-9	90
2	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	90
3	1-Heneicosyl formate	340	C22H44O2	077899-03-7	90
4	1-Hexacosanol	382	C26H54O	000506-52-5	86
5	Triacontan-15-ol	438	C30H62O	031849-26-0	83





Tentatively Identified Compound (LSC) summary

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					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2-Pentanone, 4-...	5.384	4.3	ng	25135	1	8.357	116986	20.0
(1R,2S,6S,7S,8S...	14.913	3.5	ng	43834	3	14.971	247653	20.0
Benzophenone	16.311	3.2	ng	40077	3	14.971	247653	20.0
Cinnamyl cinnamate	21.416	10.6	ng	192826	5	22.021	362953	20.0
1-Heptacosanol	21.580	3.0	ng	53921	5	22.021	362953	20.0