LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG052423\
Data File : BG057534.D
Acq On : 24 May 2023 14:00
Operator : CG/JU
Sample : 02867-21
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TP14

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: BG057534.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.391	308	315	322	rBV	11132	17751	1.88%	0.356%
2	5.879	391	398	412	rVB	199468	331909	35.19%	6.650%
3	7.012	585	591	596	rVB	16433	25189	2.67%	0.505%
4	7.506	668	675	688	rBV	206253	366603	38.87%	7.345%
5	8.358	814	820	828	rBV	63627	106783	11.32%	2.139%
6	9.538	1014	1021	1031	rVB	122210	218462	23.16%	4.377%
7	11.195	1296	1303	1313	rVB	80965	143937	15.26%	2.884%
8	13.598	1705	1712	1722	rBV	340704	525295	55.69%	10.524%
9	14.291	1824	1830	1834	rVB2	48054	68790	7.29%	1.378%
10	14.913	1927	1936	1941	rBV2	75864	106537	11.30%	2.134%
11	14.972	1941	1946	1953	rVB2	126513	203851	21.61%	4.084%
12	16.311	2167	2174	2180	rBV	53282	77650	8.23%	1.556%
13	16.458	2193	2199	2213	rVB	287116	456311	48.38%	9.142%
14	16.870	2263	2269	2276	rBV	17902	25060	2.66%	0.502%
15	17.715	2405	2413	2420	rBV	190174	281275	29.82%	5.635%
16	18.561	2552	2557	2564	rBV5	9872	25743	2.73%	0.516%
17	20.283	2844	2850	2855	rBV	724499	943207	100.00%	18.897%
18	21.234	3009	3012	3015	rBV4	8409	10206	1.08%	0.204%
19	21.416	3038	3043	3049	rVB	262323	360790	38.25%	7.229%
20	21.581	3067	3071	3081	rVB4	22186	43082	4.57%	0.863%
21	22.021	3140	3146	3153	rBV	191592	325601	34.52%	6.524%
22	25.528	3733	3743	3754	rVB	110683	327168	34.69%	6.555%

Sum of corrected areas: 4991200

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Instrument :
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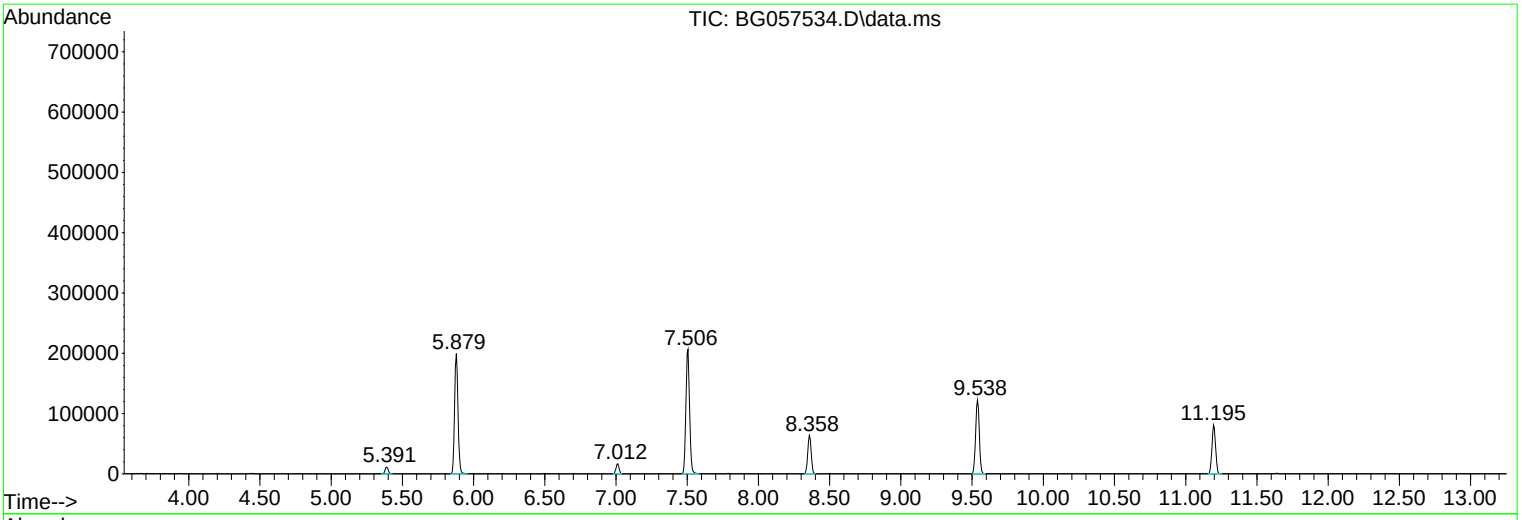
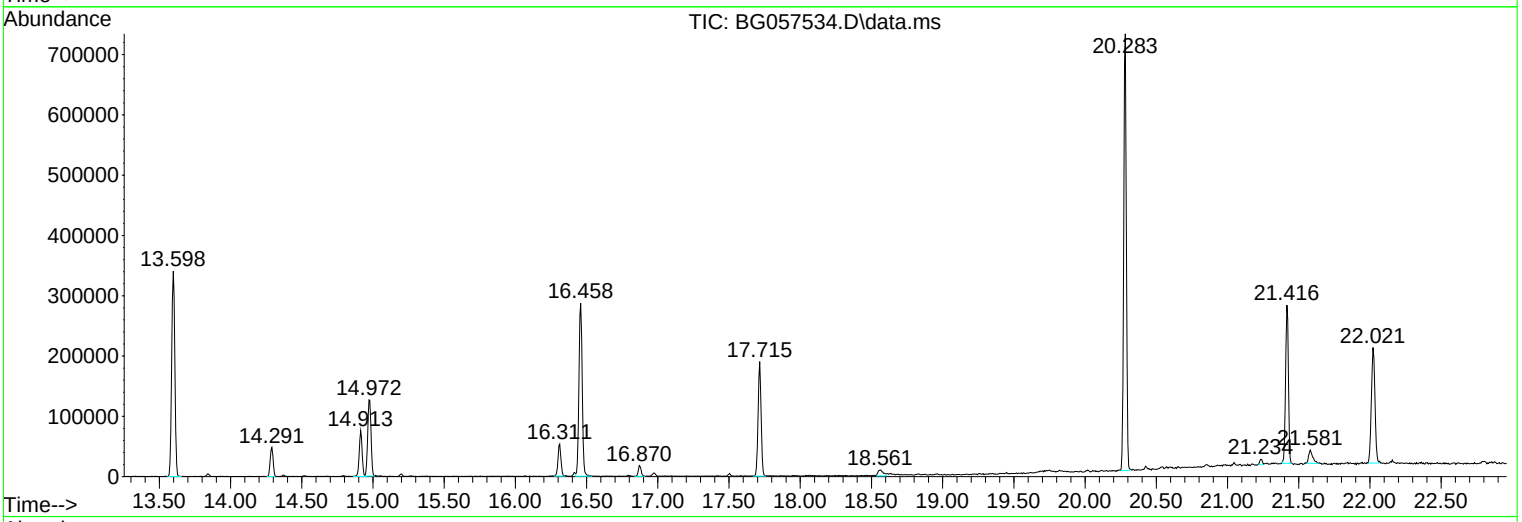
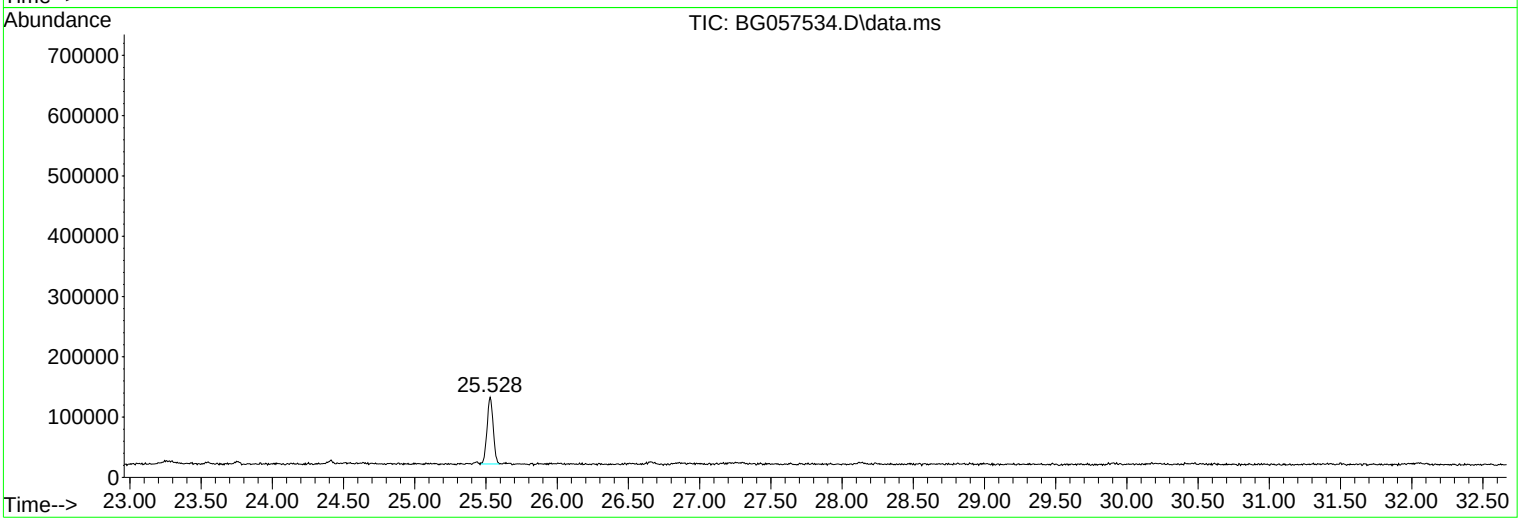
ClientSampleId :
TP14

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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Data File : BG057534.D
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Operator : CG/JU
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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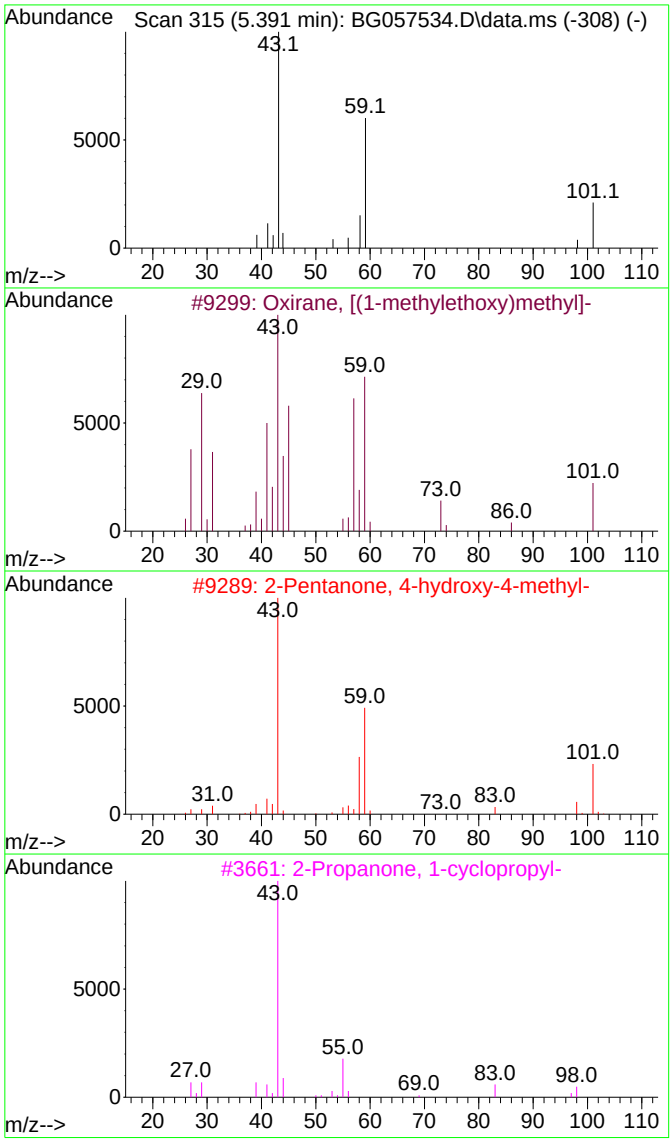
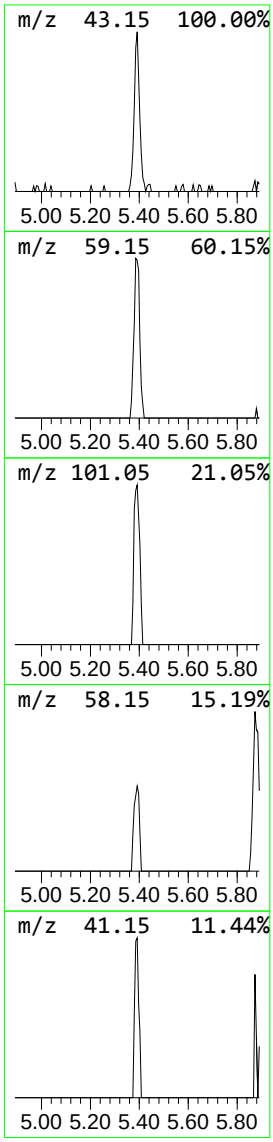
Peak Number 1 unknown5.391 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.391	3.32 ng	17751	1,4-Dichlorobenzene-d4	8.358

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oxirane, [(1-methylethoxy)methyl]-	116	C6H12O2	004016-14-2	43
2	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	39
3	2-Propanone, 1-cyclopropyl-	98	C6H10O	004160-75-2	9
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	7





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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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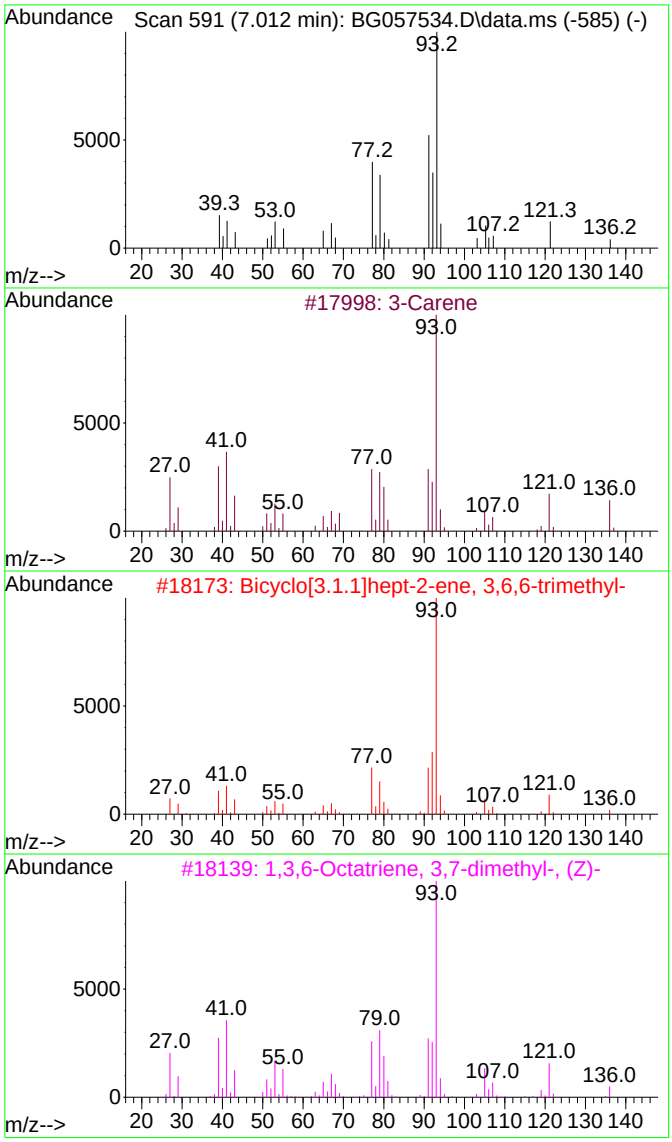
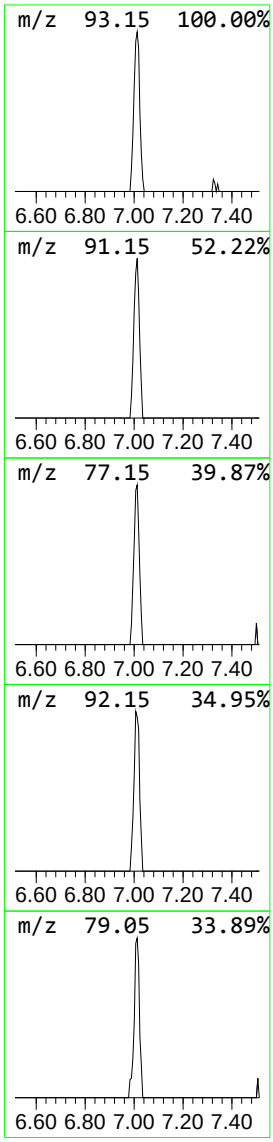
Peak Number 2 3-Carene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.012	4.72 ng	25189	1,4-Dichlorobenzene-d4	8.358

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Carene	136	C10H16	013466-78-9	91
2	Bicyclo[3.1.1]hept-2-ene, 3,6,6-...	136	C10H16	004889-83-2	90
3	1,3,6-Octatriene, 3,7-dimethyl-,...	136	C10H16	003338-55-4	87
4	trans-.beta.-Ocimene	136	C10H16	003779-61-1	86
5	.alpha.-Pinene	136	C10H16	000080-56-8	83





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Data File : BG057534.D
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Operator : CG/JU
Sample : 02867-21
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TP14

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG042723.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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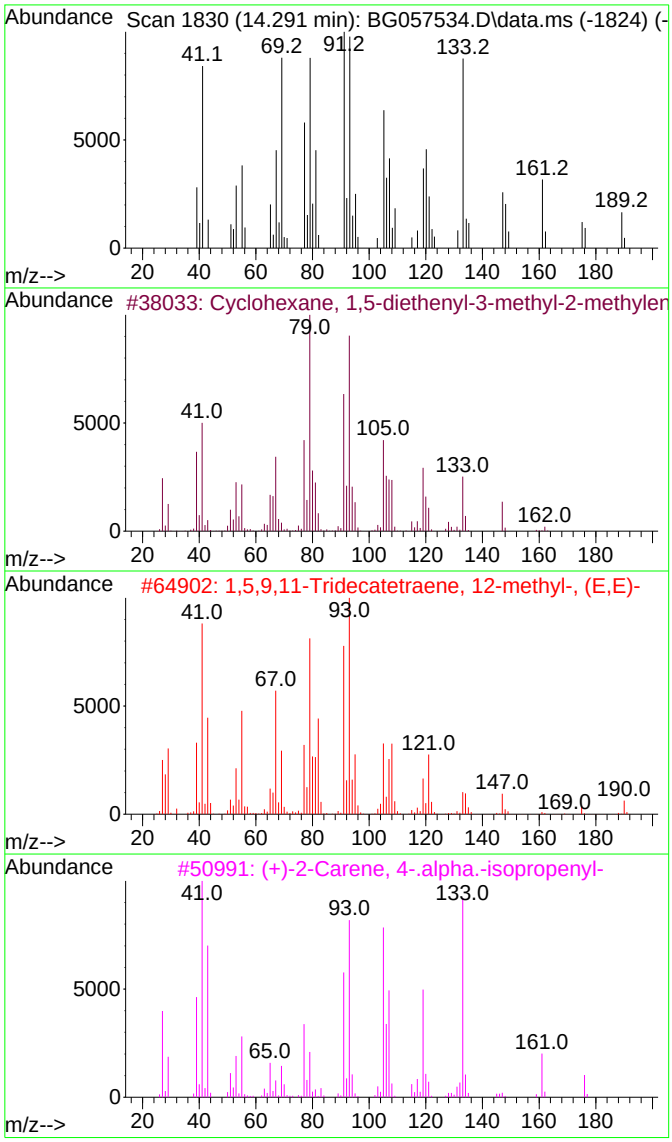
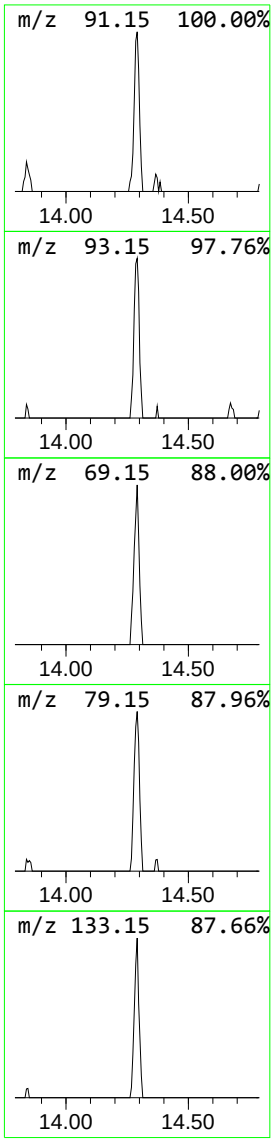
Peak Number 3 unknown14.291 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.291	6.75 ng	68790	Acenaphthene-d10	14.972

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexane, 1,5-diethenyl-3-met...	162	C12H18	074742-35-1	43
2	1,5,9,11-Tridecatetraene, 12-met...	190	C14H22	062338-27-6	42
3	(+)-2-Carene, 4-.alpha.-isoprope...	176	C13H20	1000151-26-0	42
4	Spiro[4.4]nona-1,3-diene, 1,2-di...	148	C11H16	1000163-57-6	30
5	2-Methyl-1-phenyl-2-propen-1-ol	148	C10H12O	004383-08-8	25





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Sample : 02867-21
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TP14

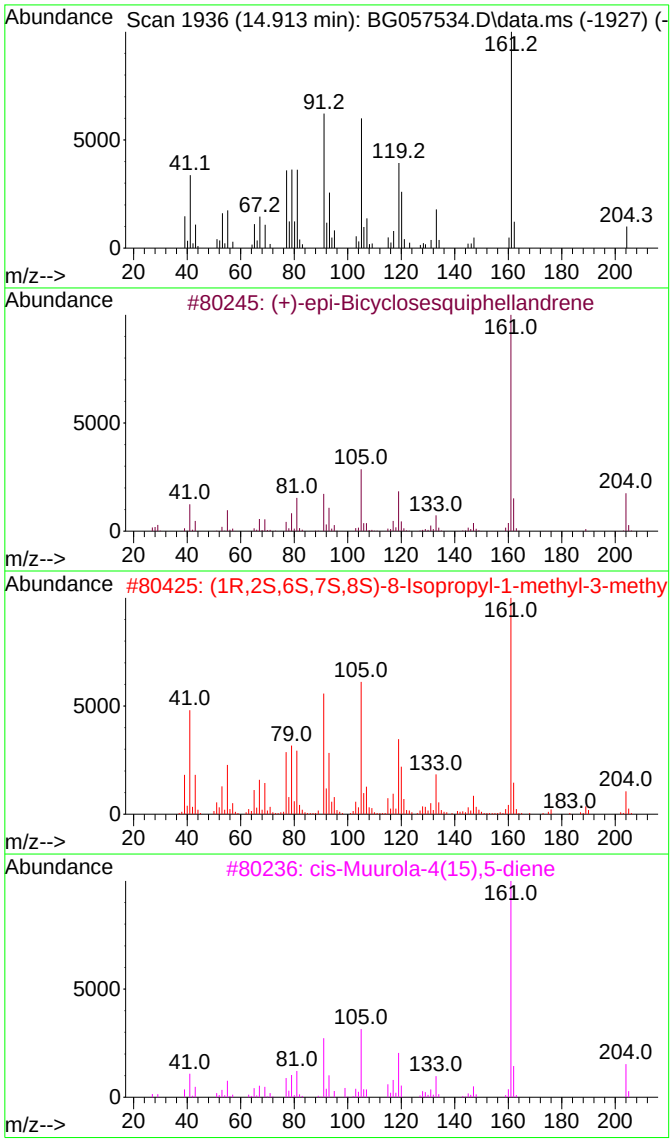
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG042723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

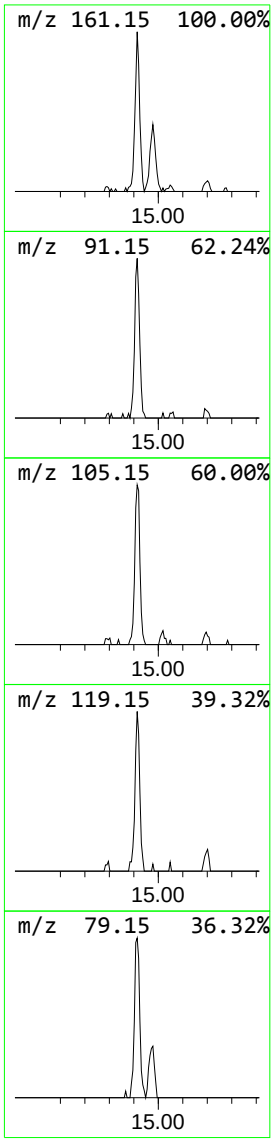
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 (+)-epi-Bicyclosesquiphella... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.913	10.45 ng	106537	Acenaphthene-d10	14.972

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(+)-epi-Bicyclosesquiphellandrene	204	C15H24	054274-73-6	91
2	(1R,2S,6S,7S,8S)-8-Isopropyl-1-m...	204	C15H24	018252-44-3	91
3	cis-Muurola-4(15),5-diene	204	C15H24	157477-72-0	86
4	1H-Cyclopenta[1,3]cyclopropa[1,2...	204	C15H24	013744-15-5	76
5	Bicyclosesquiphellandrene	204	C15H24	054324-03-7	72





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Data File : BG057534.D
Acq On : 24 May 2023 14:00
Operator : CG/JU
Sample : 02867-21
Misc :
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Instrument :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG042723.M
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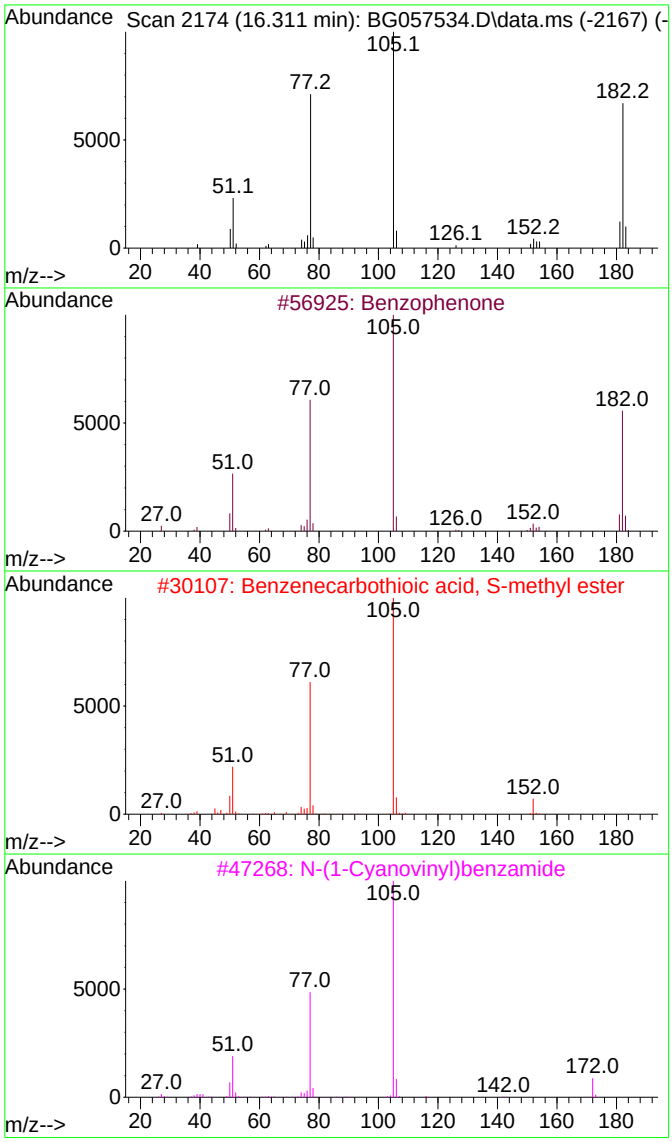
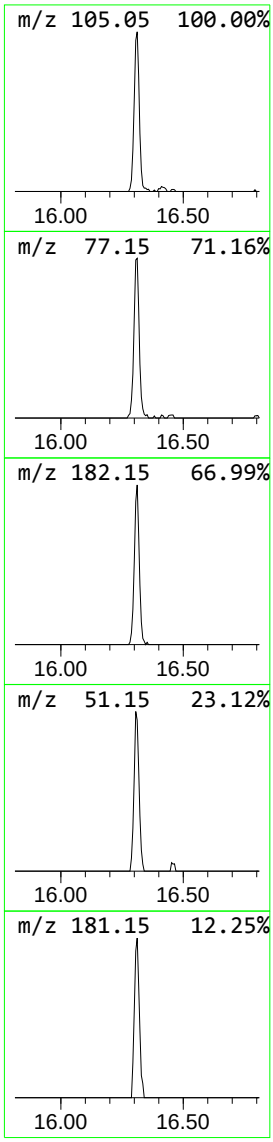
Peak Number 5 Benzophenone Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.311	7.62 ng	77650	Acenaphthene-d10	14.972

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	97
2	Benzenecarbothioic acid, S-methy...	152	C8H8OS	005925-68-8	47
3	N-(1-Cyanovinyl)benzamide	172	C10H8N2O	1000186-19-1	43
4	Vinyl benzoate	148	C9H8O2	000769-78-8	43
5	Pentafluoroethyl phenyl ketone	224	C9H5F5O	000394-52-5	43





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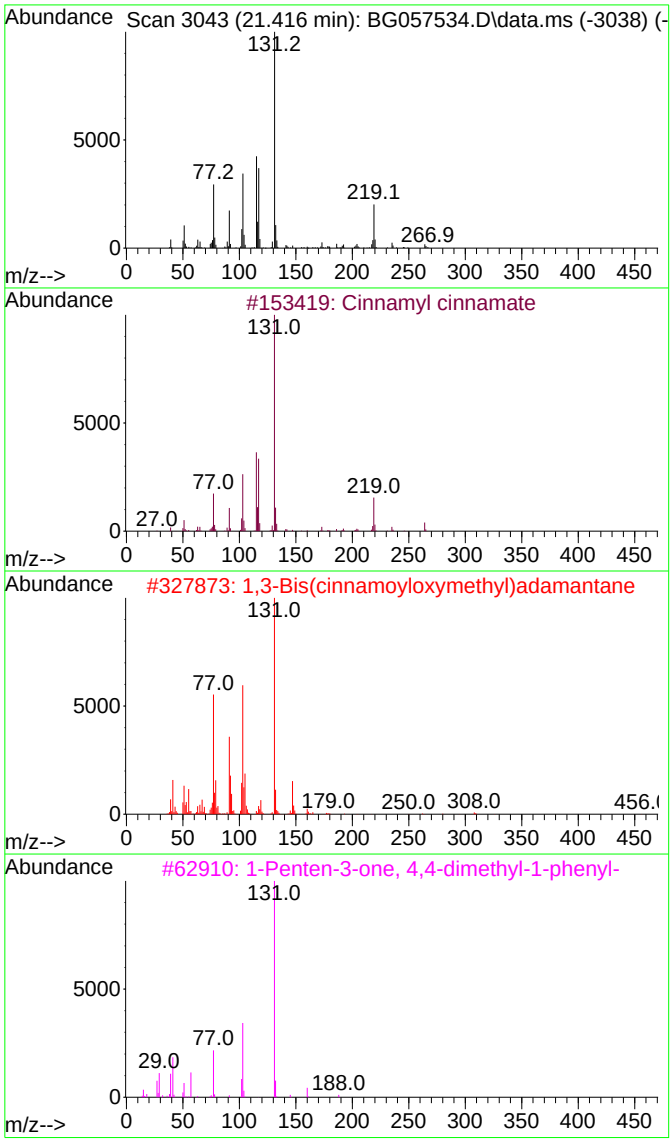
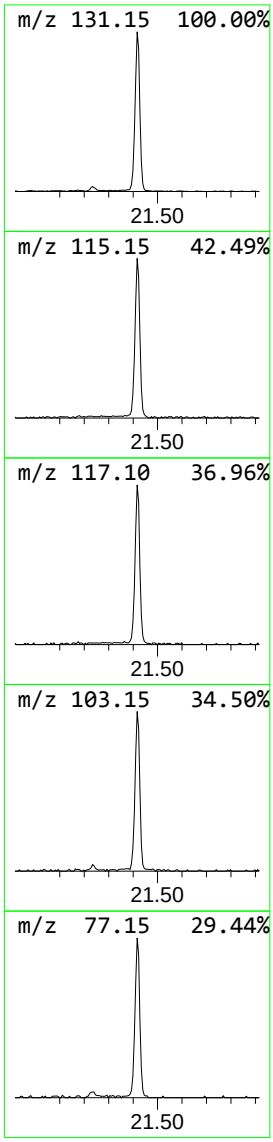
****

Peak Number 6 Cinnamyl cinnamate Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.416	22.16 ng	360790	Chrysene-d12	22.021

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cinnamyl cinnamate	264	C18H16O2	000122-69-0	91
2	1,3-Bis(cinnamoyloxymethyl)adama...	456	C30H32O4	303797-58-2	43
3	1-Penten-3-one, 4,4-dimethyl-1-p...	188	C13H16O	000538-44-3	43
4	N-(3-Chlorophenyl)-3-phenyl-2-pr...	353	C17H11ClF3NO2	1000492-37-1	43
5	2,2-Dimethyl-1-(2-vinylphenyl)pr...	188	C13H16O	1000210-99-9	43





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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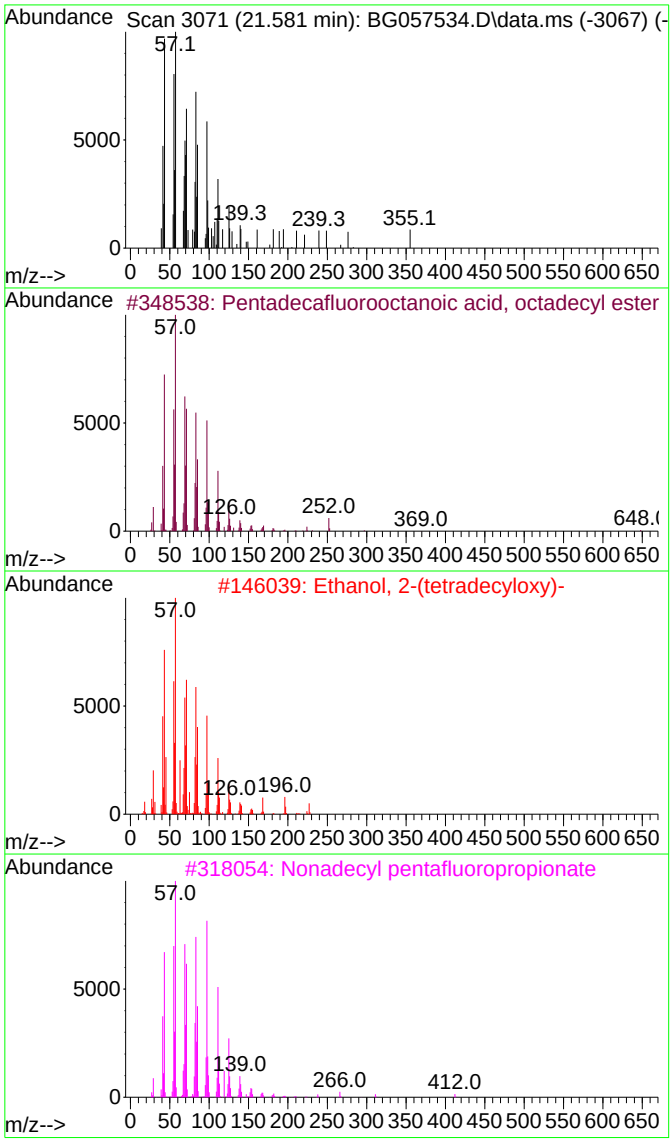
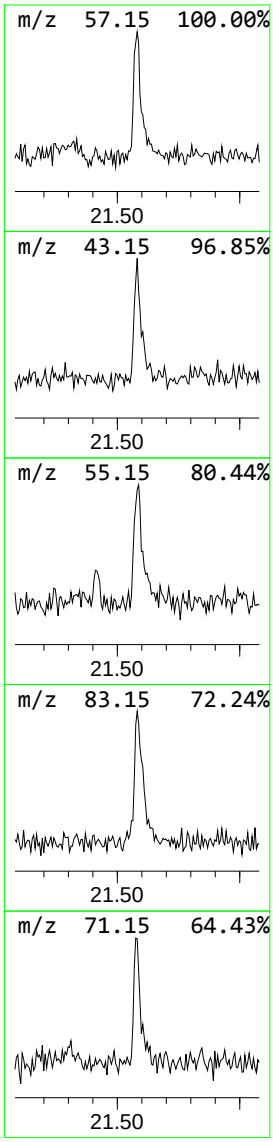
****
Peak Number 7 Pentadecafluorooctanoic aci... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.581	2.65 ng	43082	Chrysene-d12	22.021

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	90
2	Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	87
3	Nonadecyl pentafluoropropionate	430	C22H39F5O2	1000351-88-8	87
4	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	83
5	Hexadecyl propyl ether	284	C19H40O	1000406-27-9	83





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
unknown5.391	5.391	3.3	ng	17751	1	8.358	106783	20.0
3-Carene	7.012	4.7	ng	25189	1	8.358	106783	20.0
unknown14.291	14.291	6.8	ng	68790	3	14.972	203851	20.0
(+)-epi-Bicyclo...	14.913	10.4	ng	106537	3	14.972	203851	20.0
Benzophenone	16.311	7.6	ng	77650	3	14.972	203851	20.0
Cinnamyl cinnamate	21.416	22.2	ng	360790	5	22.021	325601	20.0
Pentadecafluoro...	21.581	2.6	ng	43082	5	22.021	325601	20.0