LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG020923\
Data File : BG056600.D
Acq On : 9 Feb 2023 16:52
Operator : CG/JU
Sample : 01508-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
RS-1

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-BG012723.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG056600.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.298	335	342	351	rVB	91928	145693	7.86%	1.656%
2	5.791	418	426	438	rBV	366400	621341	33.50%	7.062%
3	7.419	693	703	718	rBV	370219	658933	35.53%	7.490%
4	8.265	840	847	854	rVB	121132	207136	11.17%	2.354%
5	9.440	1039	1047	1057	rVB	229831	412795	22.26%	4.692%
6	11.097	1323	1329	1336	rVB	167873	294840	15.90%	3.351%
7	11.567	1404	1409	1415	rBV5	15669	27414	1.48%	0.312%
8	12.066	1489	1494	1499	rBV6	11467	18964	1.02%	0.216%
9	12.119	1499	1503	1508	rVV3	18143	29729	1.60%	0.338%
10	12.172	1508	1512	1519	rVB7	11598	24953	1.35%	0.284%
11	12.343	1534	1541	1547	rBV5	34627	68181	3.68%	0.775%
12	12.454	1557	1560	1567	rVB7	9865	21138	1.14%	0.240%
13	12.677	1594	1598	1607	rVB8	13689	32608	1.76%	0.371%
14	12.801	1615	1619	1622	rBV4	14149	18759	1.01%	0.213%
15	13.089	1664	1668	1676	rBV4	9980	25624	1.38%	0.291%
16	13.336	1706	1710	1714	rVB4	25288	38103	2.05%	0.433%
17	13.506	1733	1739	1749	rBV	842327	1330583	71.74%	15.124%
18	13.676	1762	1768	1775	rVB4	69810	146564	7.90%	1.666%
19	14.299	1870	1874	1882	rBV2	77789	148591	8.01%	1.689%
20	14.622	1924	1929	1933	rBV3	79090	130793	7.05%	1.487%
21	14.663	1933	1936	1939	rVV4	36129	50166	2.70%	0.570%
22	14.705	1939	1943	1947	rVB2	68681	96738	5.22%	1.100%
23	14.887	1969	1974	1980	rVB	276699	446134	24.05%	5.071%
24	15.656	2102	2105	2112	rVB3	65518	107508	5.80%	1.222%
25	16.220	2199	2201	2206	rVB	55369	73798	3.98%	0.839%
26	16.373	2221	2227	2233	rBV	521064	795695	42.90%	9.044%
27	17.625	2436	2440	2445	rVB	311558	453348	24.44%	5.153%
28	20.204	2874	2879	2884	rBV	1427988	1854689	100.00%	21.081%
29	21.920	3167	3171	3177	rVB	311895	516971	27.87%	5.876%

Sum of corrected areas: 8797789

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG020923\
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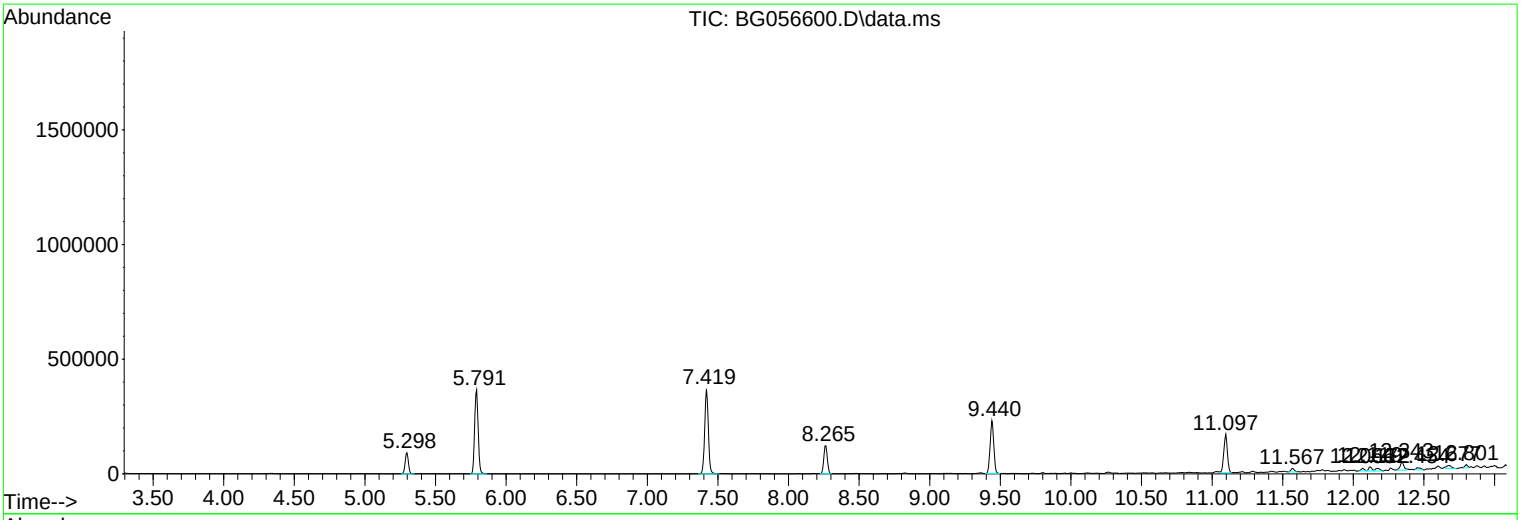
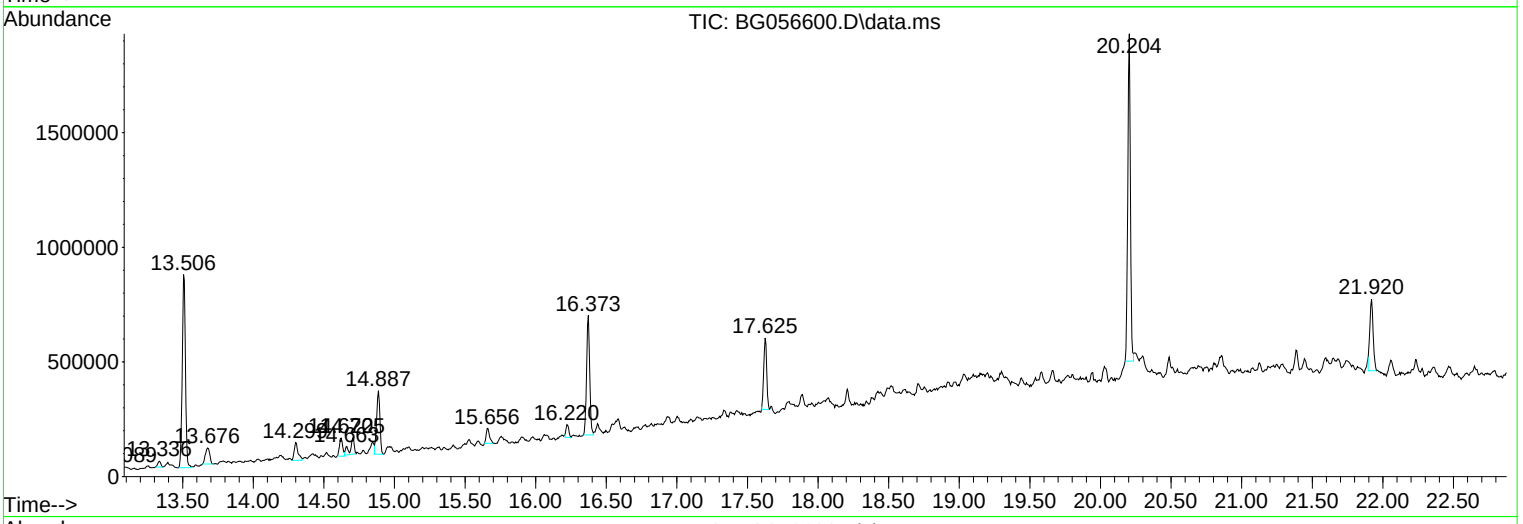
Sample : 01508-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

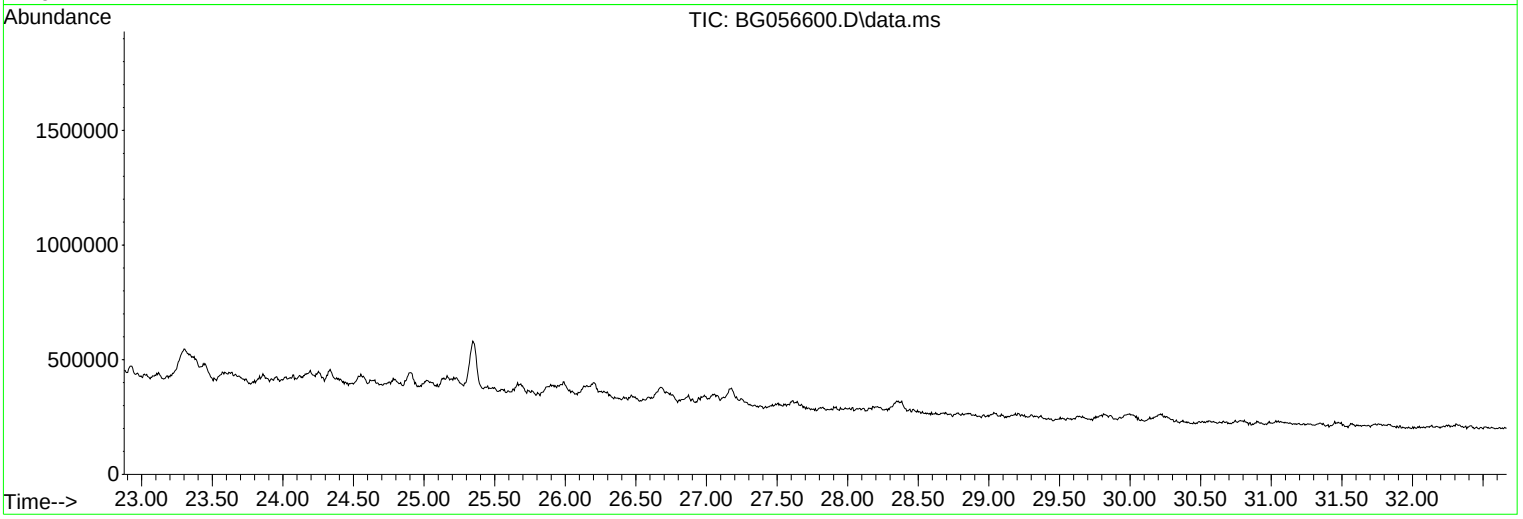
Instrument :
BNA_G
ClientSampleId :
RS-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG012723.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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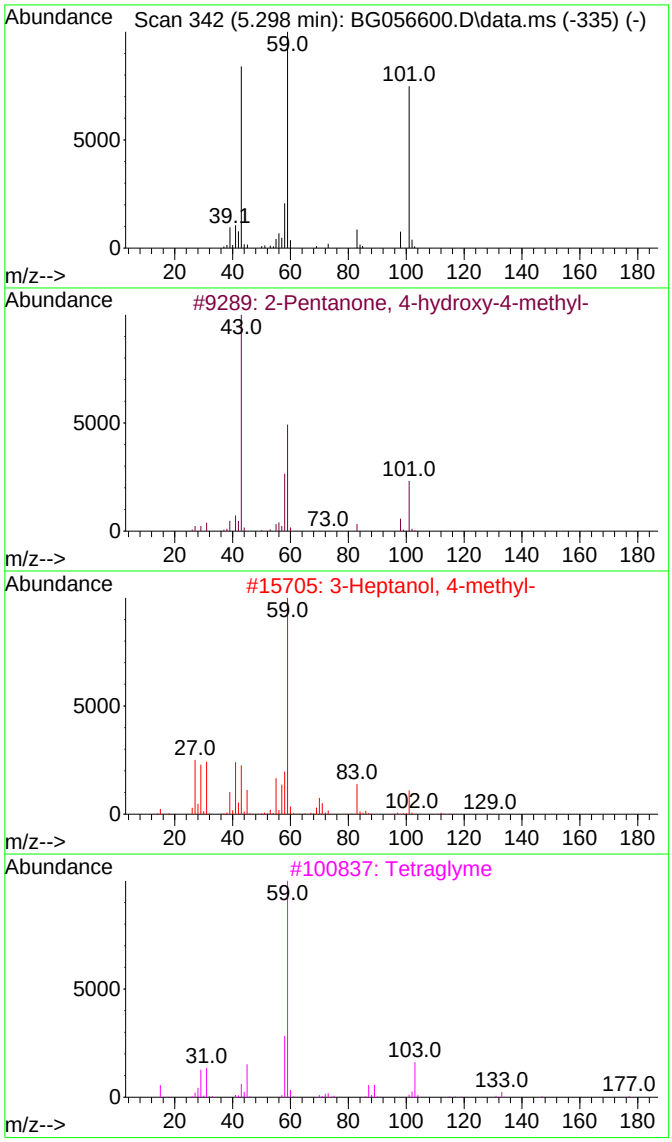
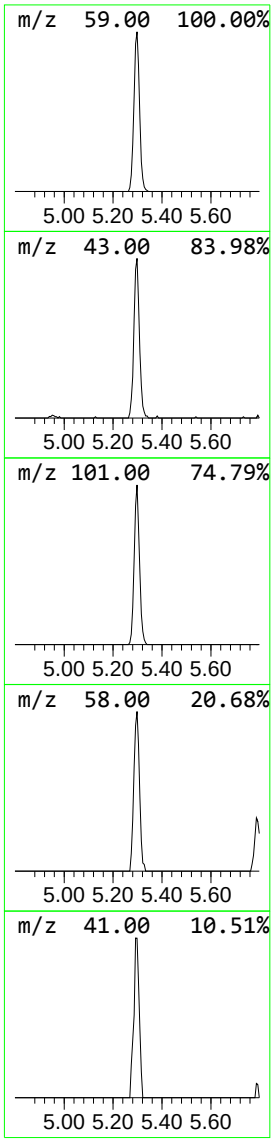
****
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.298	14.07 ng	145693	1,4-Dichlorobenzene-d4	8.265

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	45
2	3-Heptanol, 4-methyl-	130	C8H18O	014979-39-6	23
3	Tetraglyme	222	C10H22O5	000143-24-8	23
4	4-Hydroxy-3-hexanone	116	C6H12O2	004984-85-4	17
5	6-Nitrohexan-2-ol	147	C6H13NO3	062224-53-7	17





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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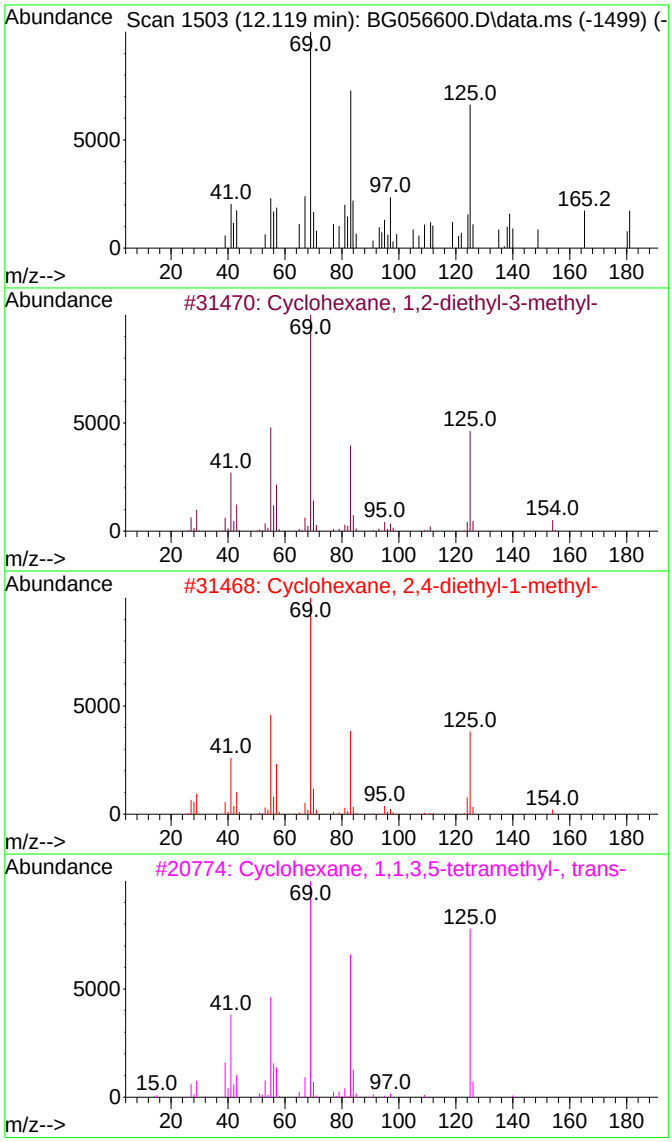
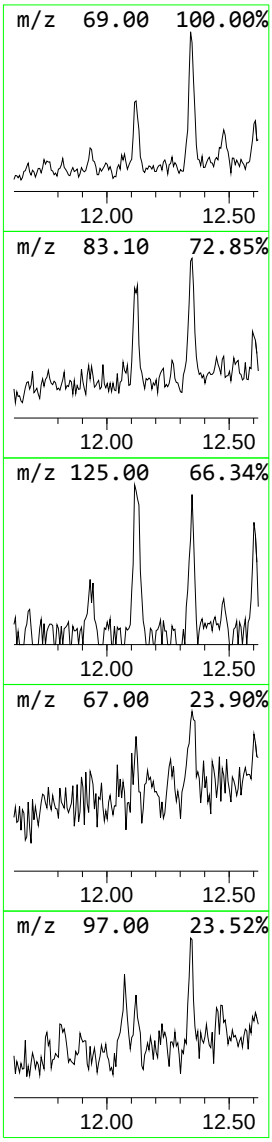
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Cyclohexane, 1,2-diethyl-3-... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.119	2.02 ng	29729	Naphthalene-d8	11.097

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexane, 1,2-diethyl-3-methyl-	154	C11H22	061141-80-8	53
2	Cyclohexane, 2,4-diethyl-1-methyl-	154	C11H22	061142-70-9	50
3	Cyclohexane, 1,1,3,5-tetramethyl...	140	C10H20	050876-31-8	50
4	2,2-Dimethyl-3-heptene trans	126	C9H18	019550-75-5	46
5	Zinc, bis[2-(1,1-dimethylethyl)-...	314	C18H34Zn	074793-36-5	43





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Operator : CG/JU
Sample : 01508-01
Misc :
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Instrument :
BNA_G
ClientSampleId :
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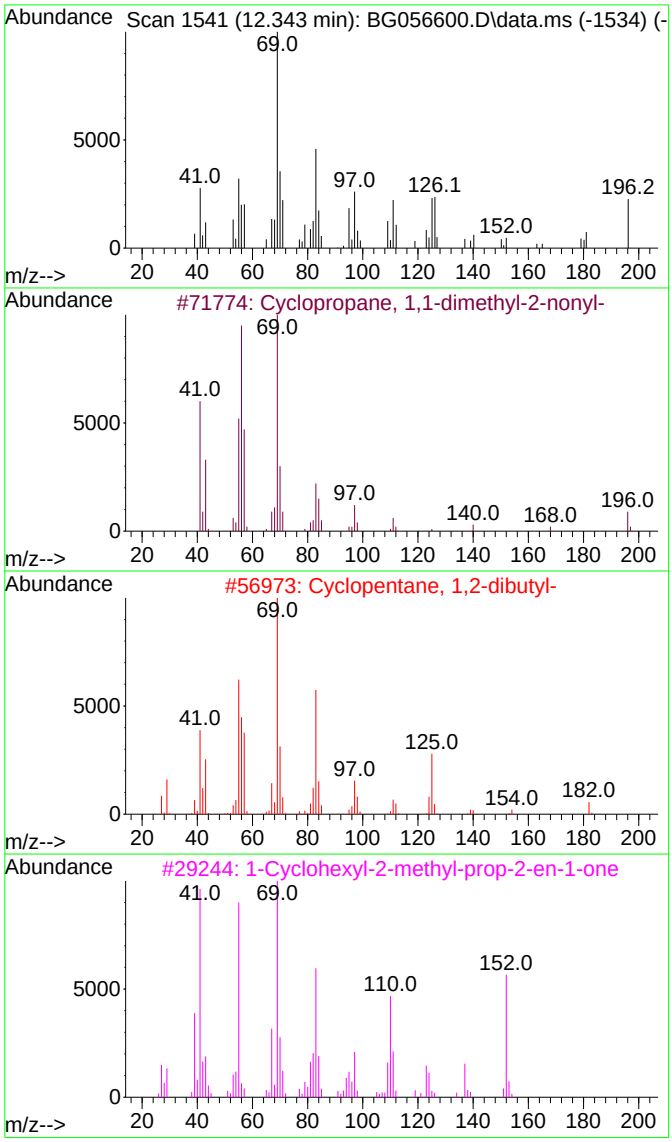
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG012723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

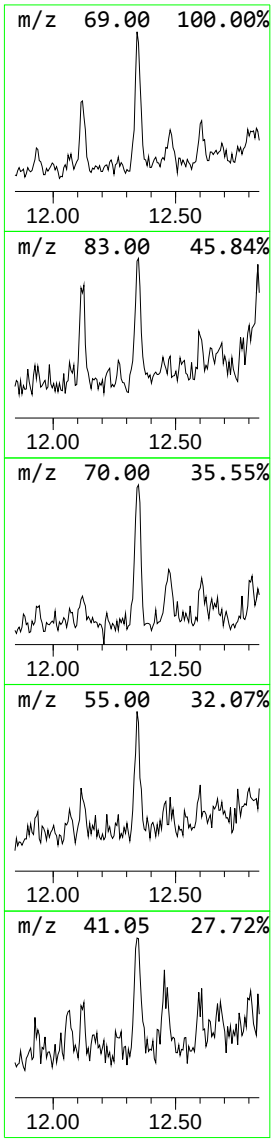
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Cyclopropane, 1,1-dimethyl-... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.343	4.62 ng	68181	Naphthalene-d8	11.097

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopropane, 1,1-dimethyl-2-nonyl-	196	C14H28	041977-38-2	53
2	Cyclopentane, 1,2-dibutyl-	182	C13H26	062199-52-4	50
3	1-Cyclohexyl-2-methyl-prop-2-en-...	152	C10H16O	025183-82-8	47
4	Cyclohexane, 1,1,2-trimethyl-	126	C9H18	007094-26-0	45
5	Cyclopentane, nonyl-	196	C14H28	002882-98-6	43





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Acq On : 9 Feb 2023 16:52
Operator : CG/JU
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Misc :
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Instrument :
BNA_G
ClientSampleId :
RS-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG012723.M
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TIC Library : C:\Database\NIST20.L
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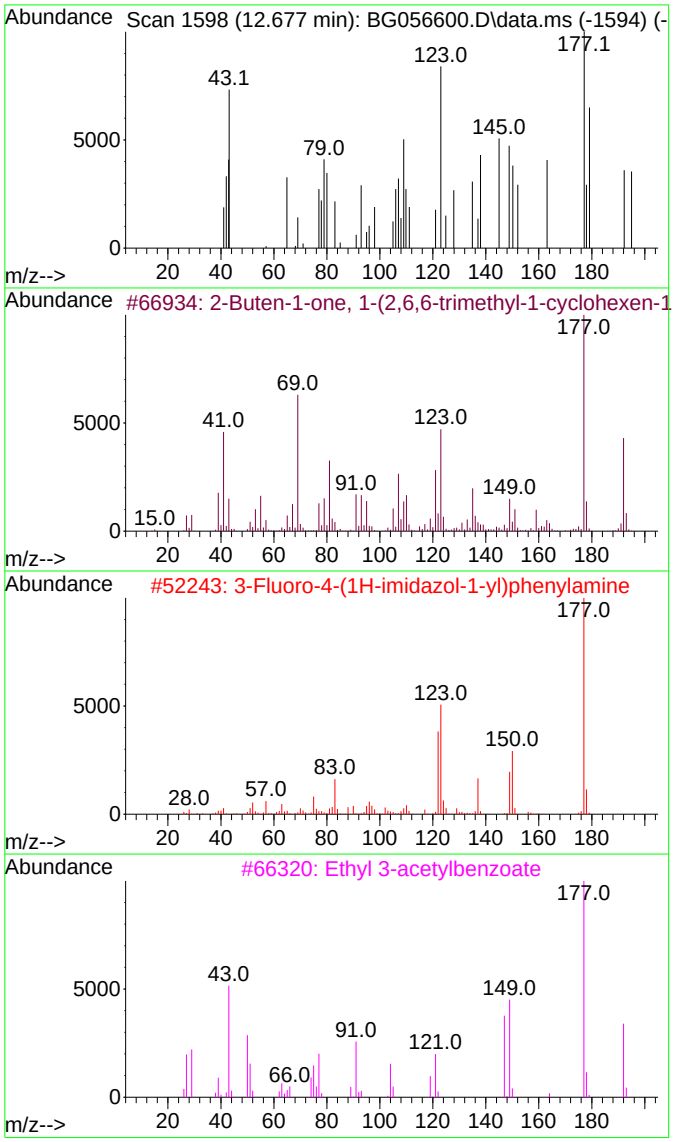
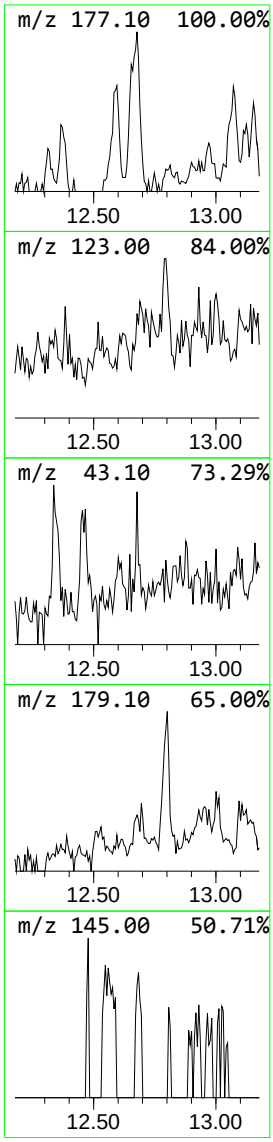
****

Peak Number 4 unknown12.678 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.678	2.21 ng	32608	Naphthalene-d8	11.097

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Buten-1-one, 1-(2,6,6-trimethy...	192	C13H20O	035044-68-9	35
2	3-Fluoro-4-(1H-imidazol-1-yl)phe...	177	C9H8FN3	190200-19-2	27
3	Ethyl 3-acetylbenzoate	192	C11H12O3	1000432-00-5	14
4	5-Ethyl-3,4-dimethyl-1H-pyrano[2...	192	C10H12N2O2	1000296-60-7	10
5	Damascone, .beta.-	192	C13H20O	023726-91-2	10





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Instrument :
BNA_G
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG012723.M
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TIC Library : C:\Database\NIST20.L
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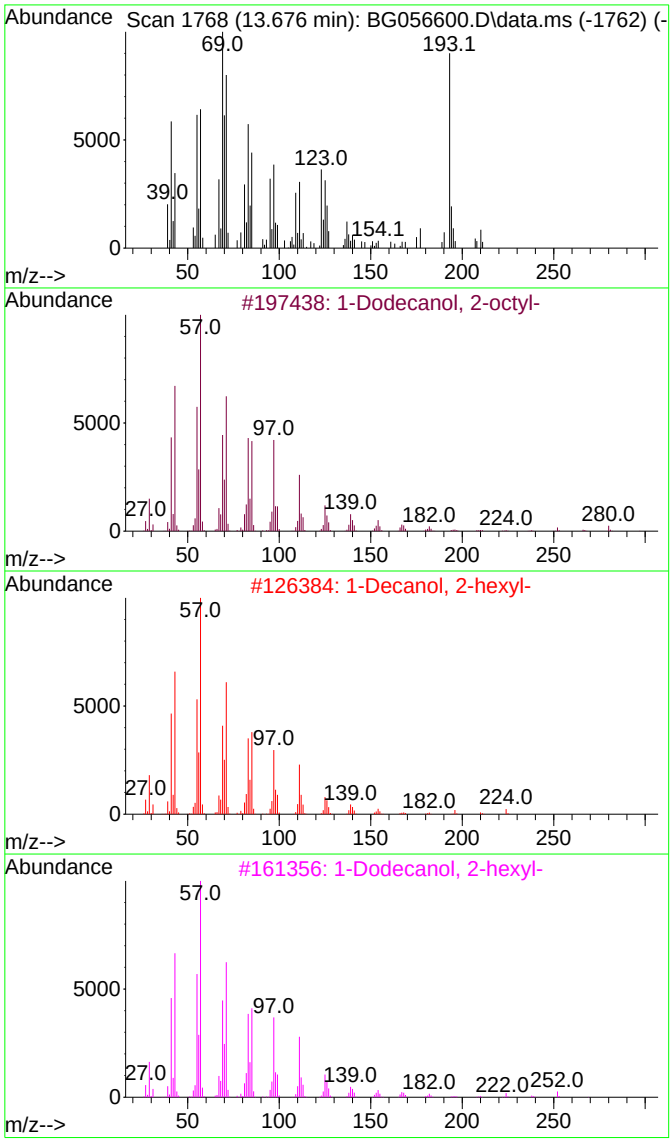
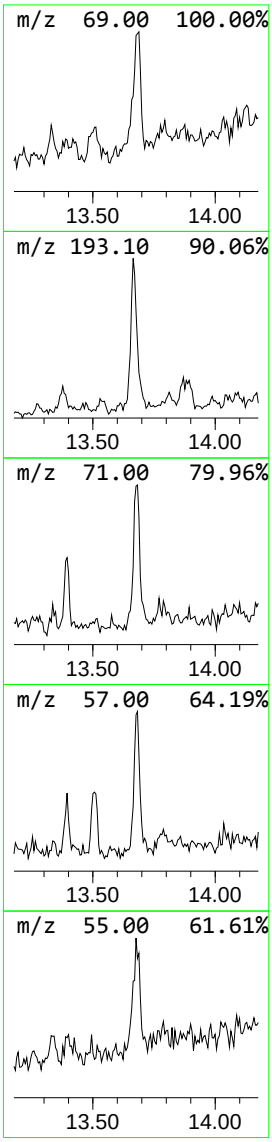
****

Peak Number 5 unknown13.676 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.676	6.57 ng	146564	Acenaphthene-d10	14.887

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Dodecanol, 2-octyl-	298	C20H42O	005333-42-6	38
2	1-Decanol, 2-hexyl-	242	C16H34O	002425-77-6	38
3	1-Dodecanol, 2-hexyl-	270	C18H38O	110225-00-8	38
4	Phosphetane, 1-chloro-2,2,3,4,4-...	194	C8H16ClOP	029276-11-7	30
5	Cyclooctane, 1,4-dimethyl-, cis-	140	C10H20	013151-99-0	25





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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG012723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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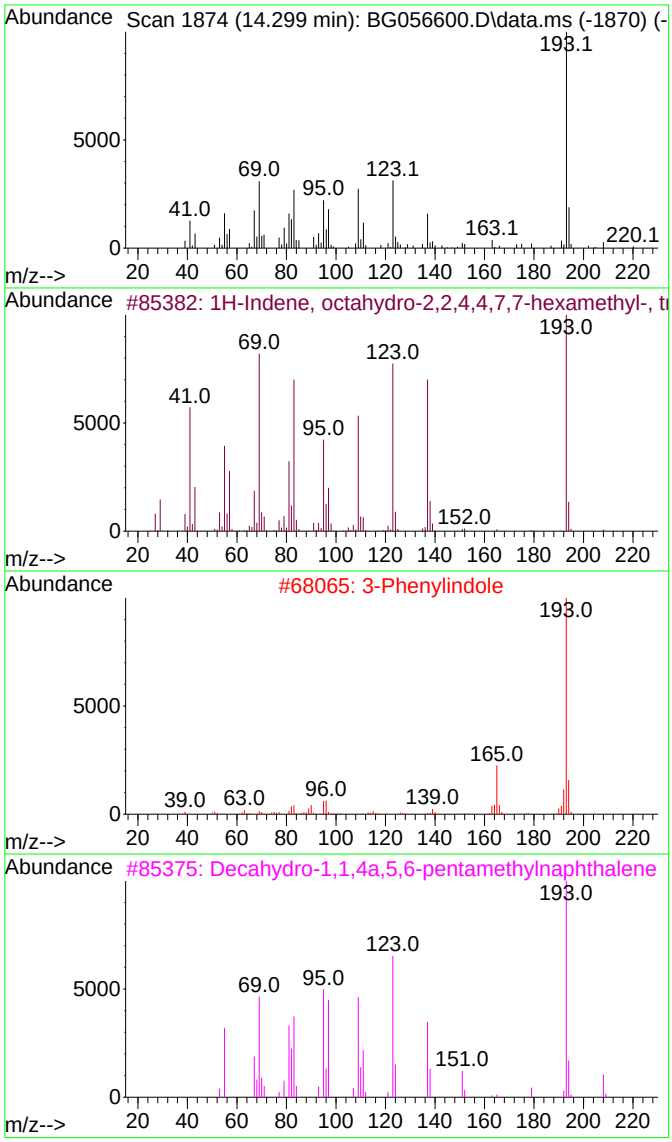
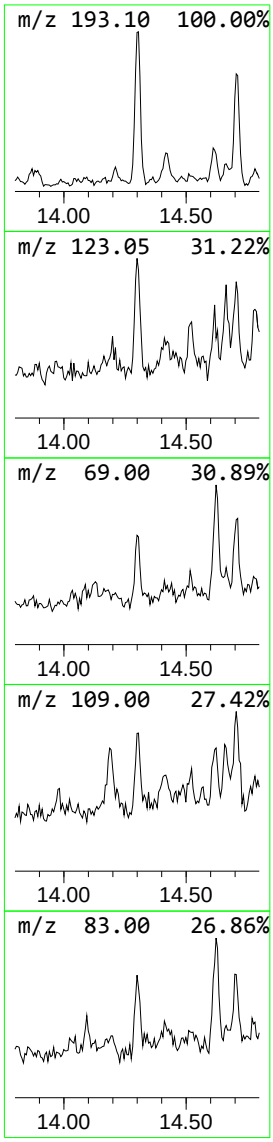
****
Peak Number 6 1H-Indene, octahydro-2,2,4,... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.299	6.66 ng	148591	Acenaphthene-d10	14.887

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Indene, octahydro-2,2,4,4,7,7...	208	C15H28	054832-83-6	72
2	3-Phenylindole	193	C14H11N	001504-16-1	47
3	Decahydro-1,1,4a,5,6-pentamethyl...	208	C15H28	080655-44-3	40
4	Iminostilbene	193	C14H11N	000256-96-2	38
5	Acetylene, 1-(2-aminophenyl)-2-p...	193	C14H11N	1000380-73-4	38





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TIC Library : C:\Database\NIST20.L
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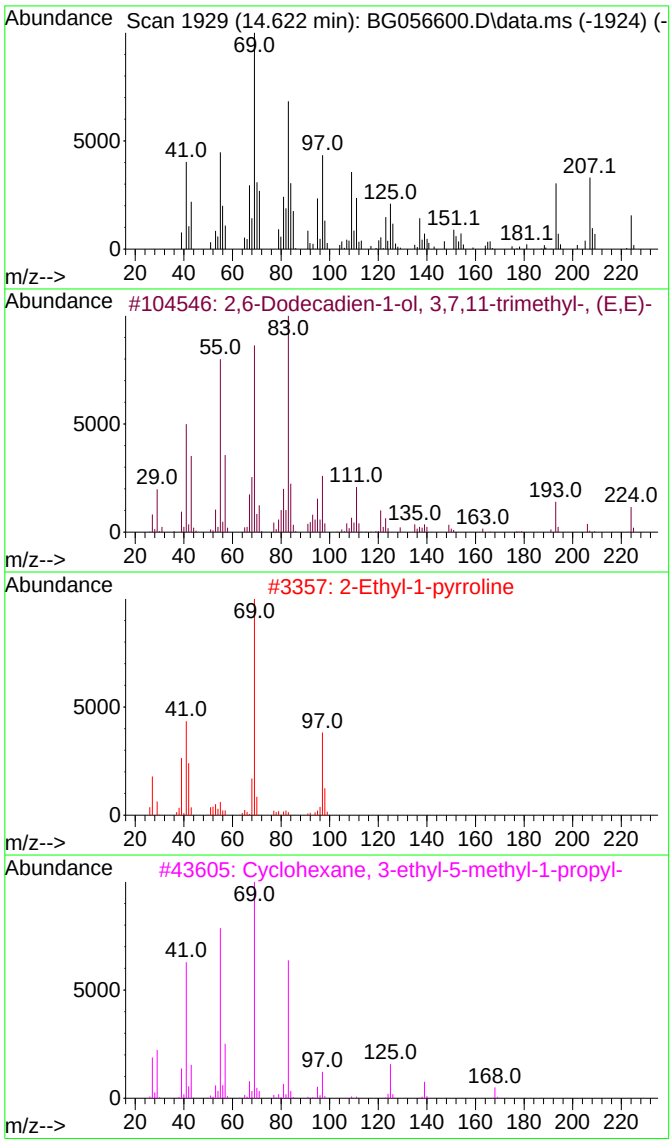
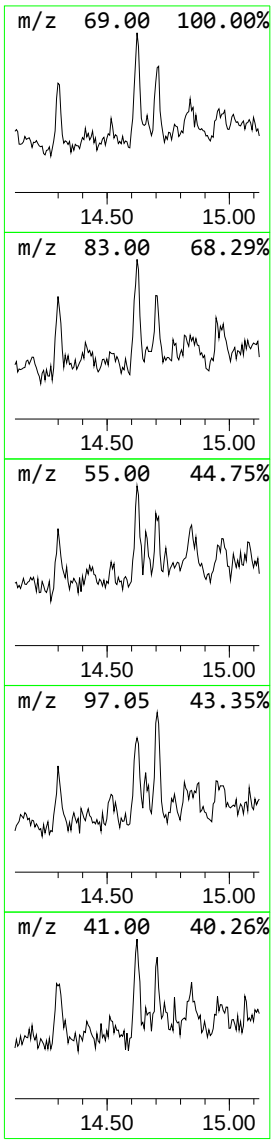
****
Peak Number 7 2,6-Dodecadien-1-ol, 3,7,11... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.622	5.86 ng	130793	Acenaphthene-d10	14.887

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,6-Dodecadien-1-ol, 3,7,11-trim...	224	C15H28O	020576-56-1	70
2	2-Ethyl-1-pyrroline	97	C6H11N	1000422-81-4	38
3	Cyclohexane, 3-ethyl-5-methyl-1-...	168	C12H24	1000151-39-5	35
4	Neral	152	C10H16O	000106-26-3	35
5	Bicyclo[2.2.2]octan-1-amine	125	C8H15N	001193-42-6	35





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TIC Library : C:\Database\NIST20.L
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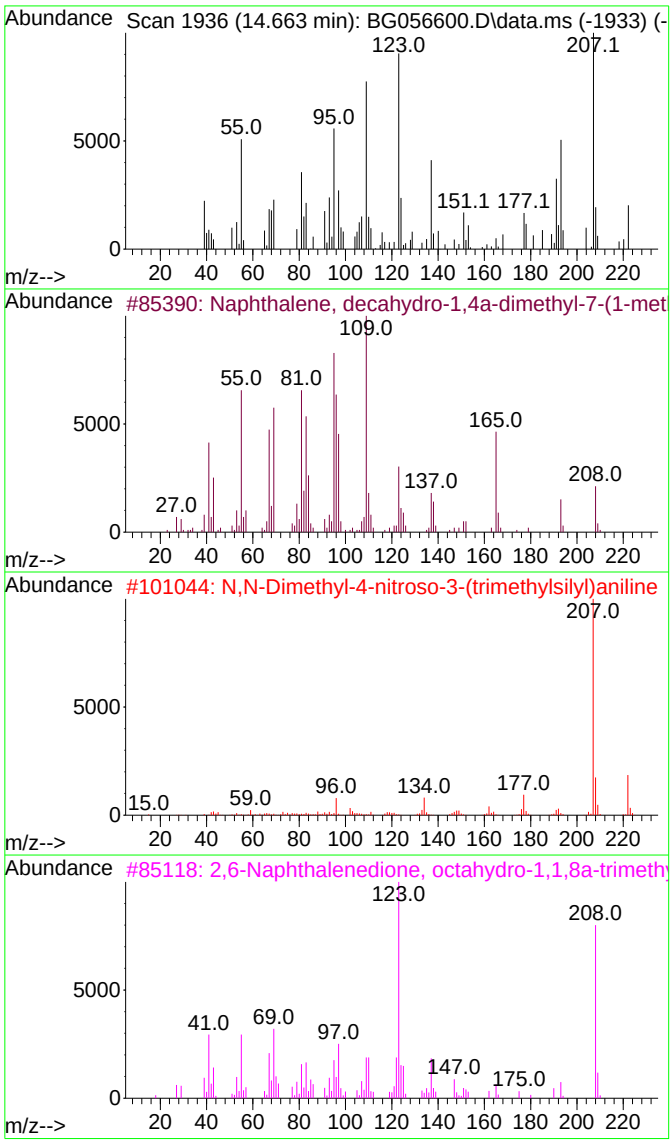
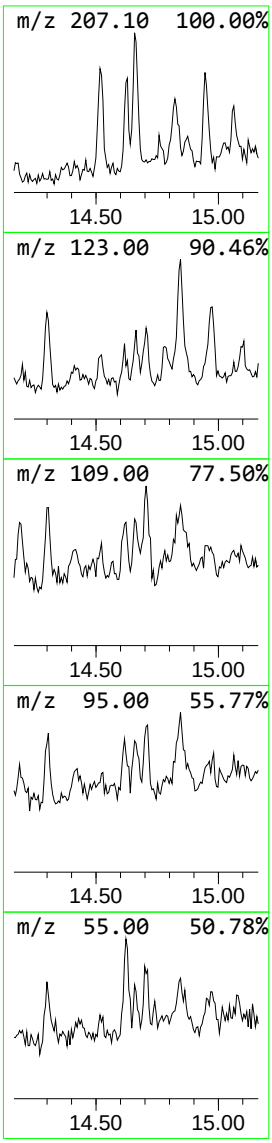
****

Peak Number 8 unknown14.663 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.663	2.25 ng	50166	Acenaphthene-d10	14.887

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, decahydro-1,4a-dime...	208	C15H28	030824-81-8	27
2	N,N-Dimethyl-4-nitroso-3-(trimet...	222	C11H18N2OSi	017993-84-9	18
3	2,6-Naphthalenedione, octahydro-...	208	C13H20O2	057289-16-4	14
4	1-(Azidomethyl)-4-fluorobenzene	151	C7H6FN3	159979-96-1	14
5	1-Cyclohexanol, 2-(3-methyl-1,3-...	208	C14H24O	1000196-01-6	14





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Operator : CG/JU
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Misc :
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Instrument :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG012723.M
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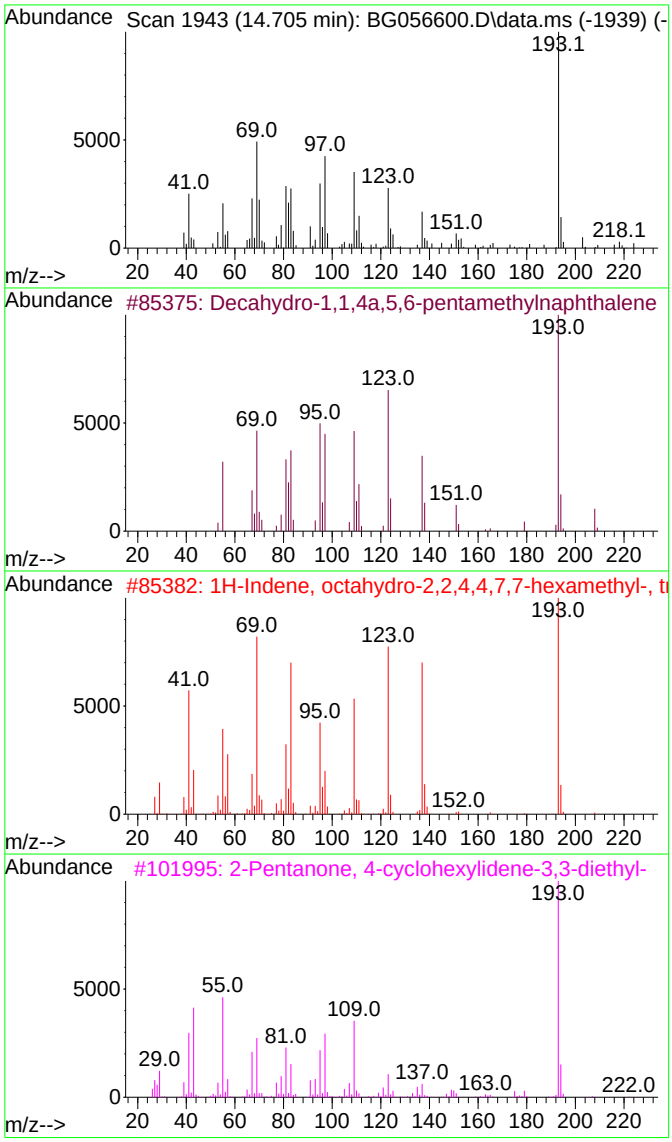
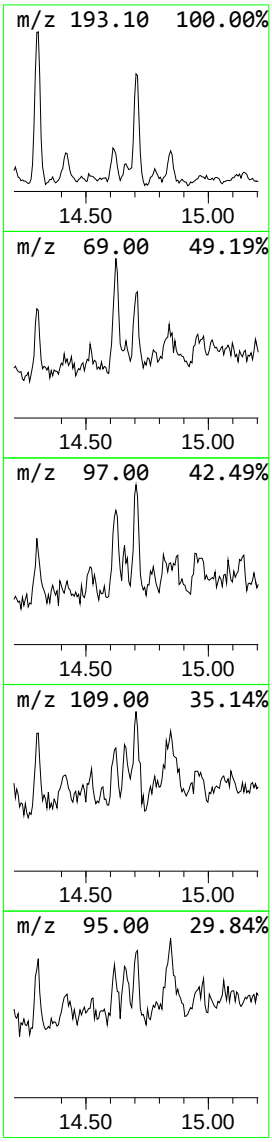
****
Peak Number 9 Decahydro-1,1,4a,5,6-pentam... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.704	4.34 ng	96738	Acenaphthene-d10	14.887

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Decahydro-1,1,4a,5,6-pentamethyl...	208	C15H28	080655-44-3	64
2	1H-Indene, octahydro-2,2,4,4,7,7...	208	C15H28	054832-83-6	55
3	2-Pentanone, 4-cyclohexylidene-3...	222	C15H26O	313253-65-5	53
4	1-Indolinecarboxaldehyde, 2-hydr...	193	C10H11NO3	013303-70-3	47
5	Silane, chlorodiethylhexyloxy-	222	C10H23ClOSi	1000363-74-4	43





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Data File : BG056600.D
Acq On : 9 Feb 2023 16:52
Operator : CG/JU
Sample : 01508-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
RS-1

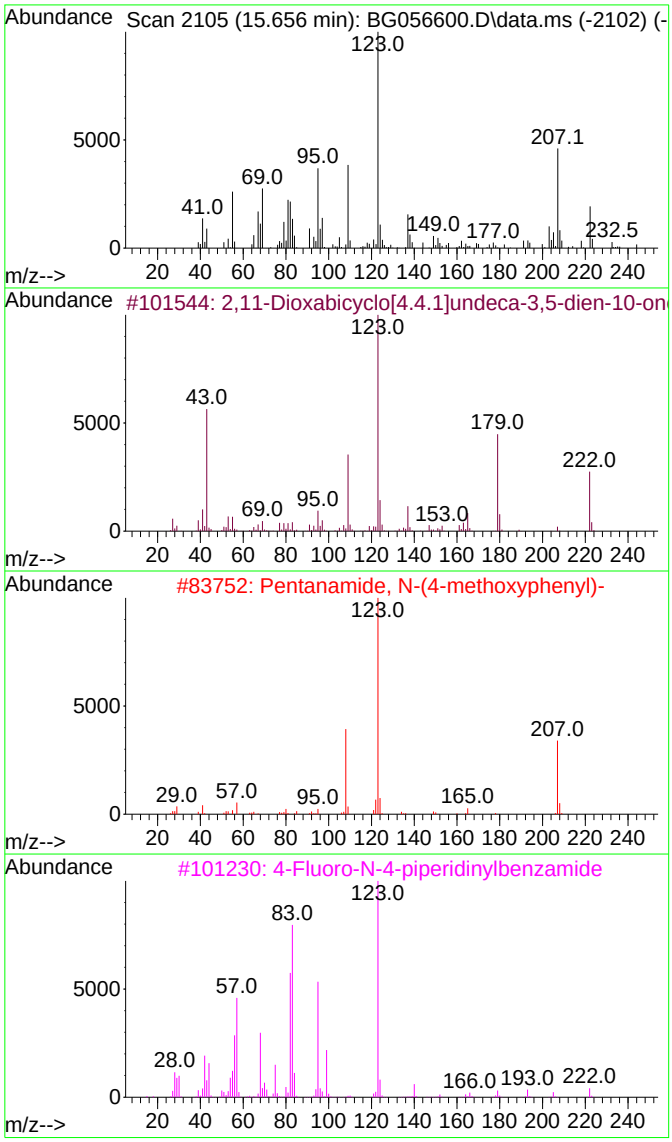
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG012723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

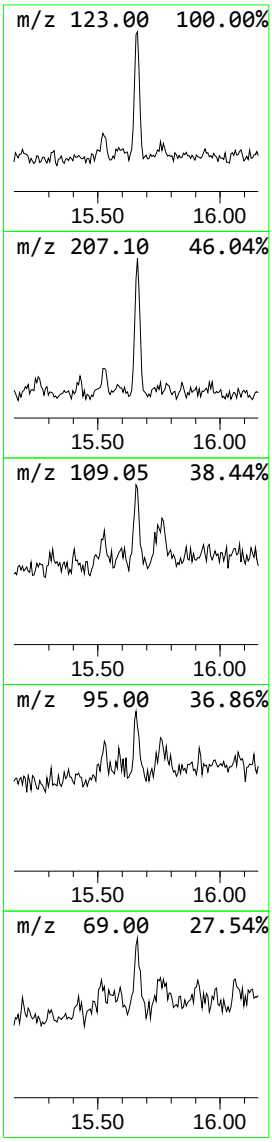
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 2,11-Dioxabicyclo[4.4.1]und... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.656	4.82 ng	107508	Acenaphthene-d10	14.887

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,11-Dioxabicyclo[4.4.1]undeca-3...	222	C13H18O3	070412-52-1	58
2	Pentanamide, N-(4-methoxyphenyl)-	207	C12H17NO2	1000306-89-3	46
3	4-Fluoro-N-4-piperidinylbenzamide	222	C12H15FN2O	075484-39-8	38
4	4-Fluoro-N-(1H-tetrazol-5-yl)ben...	207	C8H6FN5O	1000306-76-6	38
5	2-Pyrimidinamine, 4,6-dimethyl-	123	C6H9N3	000767-15-7	38





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG020923\
Data File : BG056600.D
Acq On : 9 Feb 2023 16:52
Operator : CG/JU
Sample : 01508-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
RS-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG012723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

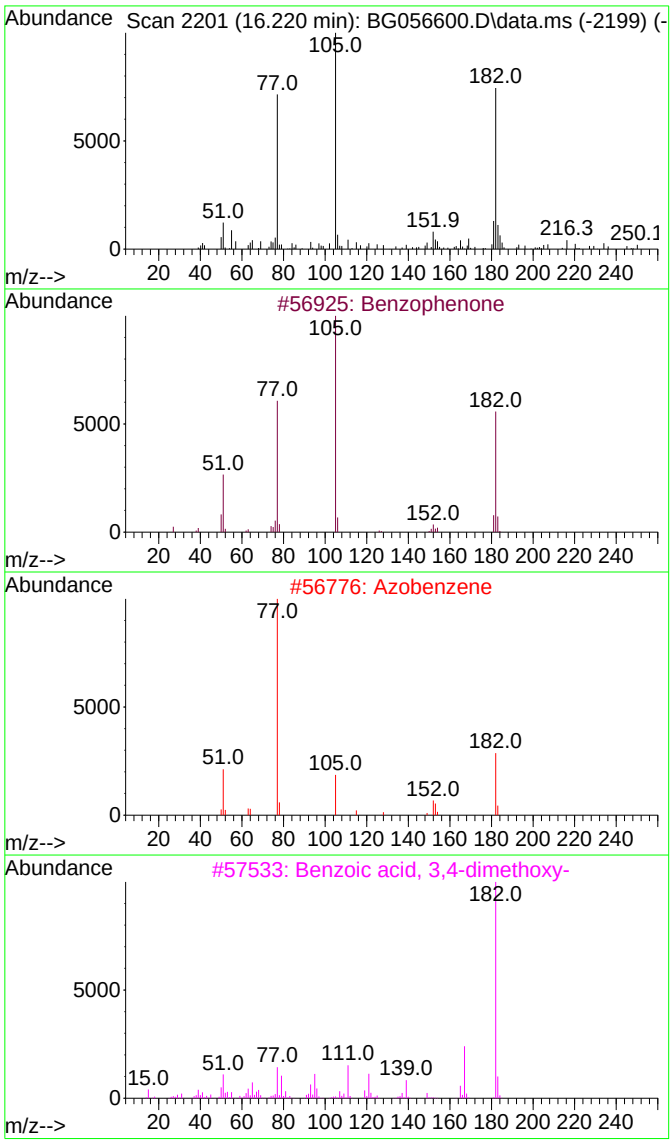
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

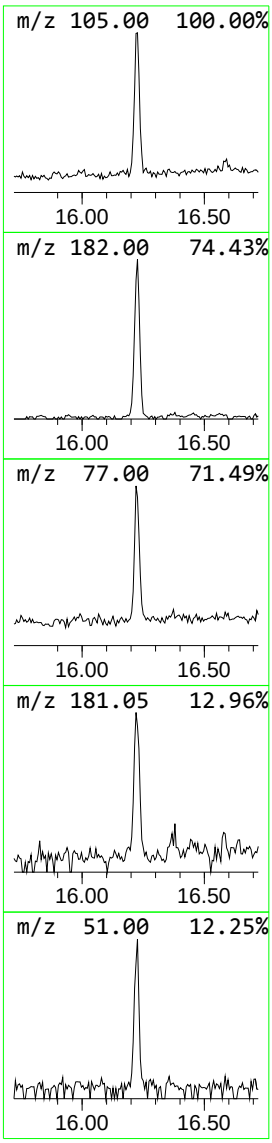
****

Peak Number 11 Benzophenone Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.220	3.31 ng	73798	Acenaphthene-d10	14.887

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	90
2	Azobenzene	182	C12H10N2	000103-33-3	72
3	Benzoic acid, 3,4-dimethoxy-	182	C9H10O4	000093-07-2	47
4	2-Methyl-1H-perimidine	182	C12H10N2	005157-10-8	46
5	3,3'-Dimethylbiphenyl	182	C14H14	000612-75-9	46





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG020923\
Data File : BG056600.D
Acq On : 9 Feb 2023 16:52
Operator : CG/JU
Sample : 01508-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
RS-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG012723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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-...	5.298	14.1	ng	145693	1	8.265	207136	20.0
Cyclohexane, 1,...	12.119	2.0	ng	29729	2	11.097	294840	20.0
Cyclopropane, 1...	12.343	4.6	ng	68181	2	11.097	294840	20.0
unknown12.678	12.678	2.2	ng	32608	2	11.097	294840	20.0
unknown13.676	13.676	6.6	ng	146564	3	14.887	446134	20.0
1H-Indene, octa...	14.299	6.7	ng	148591	3	14.887	446134	20.0
2,6-Dodecadien-...	14.622	5.9	ng	130793	3	14.887	446134	20.0
unknown14.663	14.663	2.3	ng	50166	3	14.887	446134	20.0
Decahydro-1,1,4...	14.704	4.3	ng	96738	3	14.887	446134	20.0
2,11-Dioxabicyc...	15.656	4.8	ng	107508	3	14.887	446134	20.0
Benzophenone	16.220	3.3	ng	73798	3	14.887	446134	20.0