LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG122223\
Data File : BG060144.D
Acq On : 22 Dec 2023 18:52
Operator : MA/JU
Sample : 05897-22
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
GHL-SS-27

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-BG122123.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG060144.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.156	8	11	24	rVB	144710	281536	2.50%	0.525%
2	4.443	224	230	240	rBV	276833	443730	3.94%	0.827%
3	5.042	327	332	339	rVB	78748	123629	1.10%	0.230%
4	5.512	405	412	432	rBV	1677685	2923993	25.99%	5.449%
5	7.104	675	683	701	rBV	1968442	3574289	31.77%	6.660%
6	7.939	817	825	835	rBV	429521	768228	6.83%	1.432%
7	9.102	1016	1023	1032	rBV	1003124	1818480	16.17%	3.389%
8	10.741	1293	1302	1308	rBV	740819	1364722	12.13%	2.543%
9	10.788	1308	1310	1317	rVB2	72755	129930	1.15%	0.242%
10	12.398	1579	1584	1593	rVB	112054	193726	1.72%	0.361%
11	12.621	1616	1622	1629	rBV2	102176	186347	1.66%	0.347%
12	13.197	1713	1720	1731	rBV	3865225	6064993	53.91%	11.302%
13	13.896	1832	1839	1843	rBV3	68729	130831	1.16%	0.244%
14	14.578	1944	1955	1961	rBV	1810686	2854734	25.38%	5.320%
15	14.971	2017	2022	2028	rBV2	71184	118787	1.06%	0.221%
16	15.612	2126	2131	2136	rBV2	128839	198725	1.77%	0.370%
17	16.064	2201	2208	2217	rBV	3798884	5886463	52.33%	10.969%
18	16.305	2239	2249	2258	rVB2	213638	460516	4.09%	0.858%
19	16.863	2339	2344	2351	rBV4	83856	136321	1.21%	0.254%
20	17.075	2372	2380	2383	rBV2	88566	136391	1.21%	0.254%
21	17.322	2416	2422	2428	rBV	2727140	4390191	39.03%	8.181%
22	17.815	2501	2506	2512	rBV2	105430	140917	1.25%	0.263%
23	18.215	2568	2574	2588	rBV2	472980	870094	7.73%	1.621%
24	18.509	2620	2624	2628	rBV	101241	116320	1.03%	0.217%
25	19.137	2728	2731	2737	rVB	122999	148249	1.32%	0.276%
26	19.942	2862	2868	2880	rBV	8570376	11249368	100.00%	20.962%
27	20.248	2917	2920	2924	rVB	138374	161711	1.44%	0.301%
28	20.741	3001	3004	3009	rVB	138271	150095	1.33%	0.280%
29	21.241	3084	3089	3102	rBV3	381979	667464	5.93%	1.244%
30	21.587	3142	3148	3161	rVB2	2271412	3719824	33.07%	6.932%
31	21.781	3177	3181	3185	rVB2	104643	158080	1.41%	0.295%
32	22.380	3280	3283	3290	rVB4	107141	186564	1.66%	0.348%
33	23.861	3530	3535	3542	rBV3	72064	153824	1.37%	0.287%
34	24.760	3679	3688	3702	rVB	1306570	3755603	33.39%	6.998%

Sum of corrected areas: 53664675

Instrument :
BNA_G
ClientSampleId :
GHL-SS-27

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG122223\
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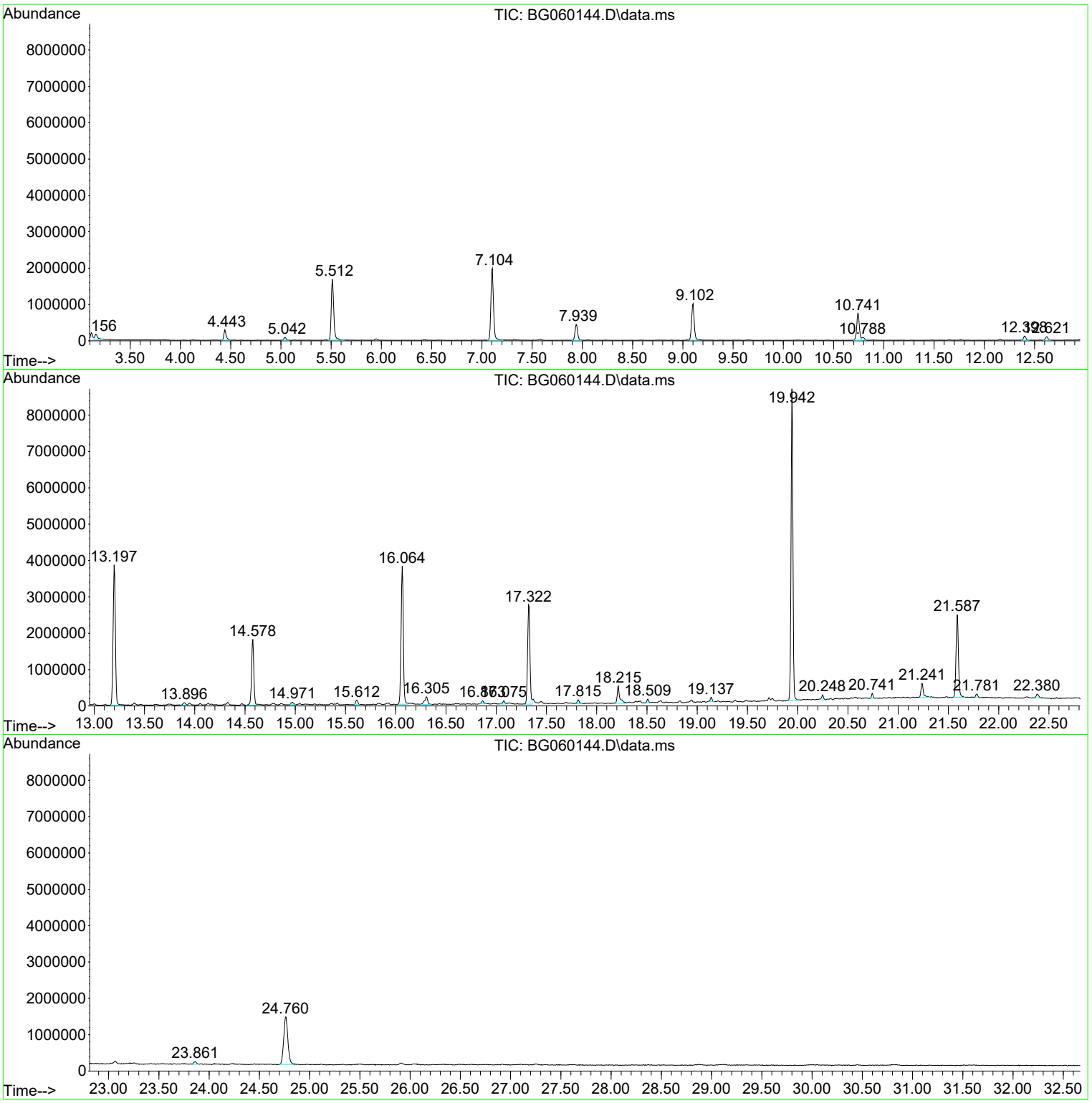
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
GHL-SS-27

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG122123.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 : BG060144.D
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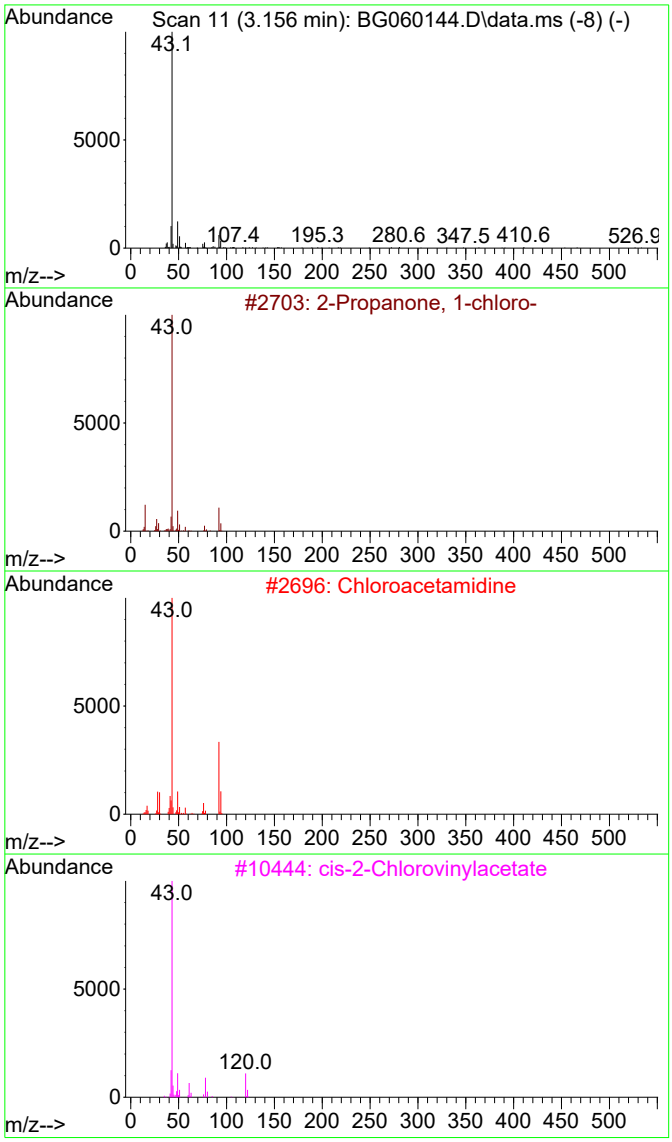
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

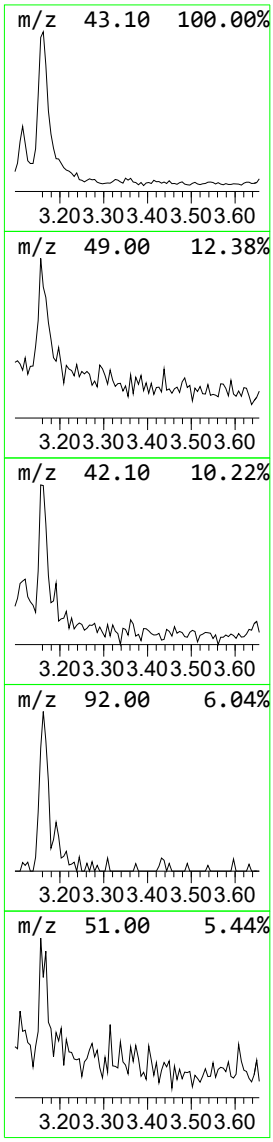
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 2-Propanone, 1-chloro- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.156	7.33 ng	281536	1,4-Dichlorobenzene-d4	7.939

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propanone, 1-chloro-	92	C3H5ClO	000078-95-5	58
2	Chloroacetamidine	92	C2H5ClN2	020846-52-0	50
3	cis-2-Chlorovinylacetate	120	C4H5ClO2	103659-54-7	9
4	Acetic acid, chloro-, 1-methylbu...	164	C7H13ClO2	090380-52-2	9
5	2-Aminoethanesulfonamide	124	C2H8N2O2S	004378-70-5	4





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Data File : BG060144.D
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Sample : 05897-22
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Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG122123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

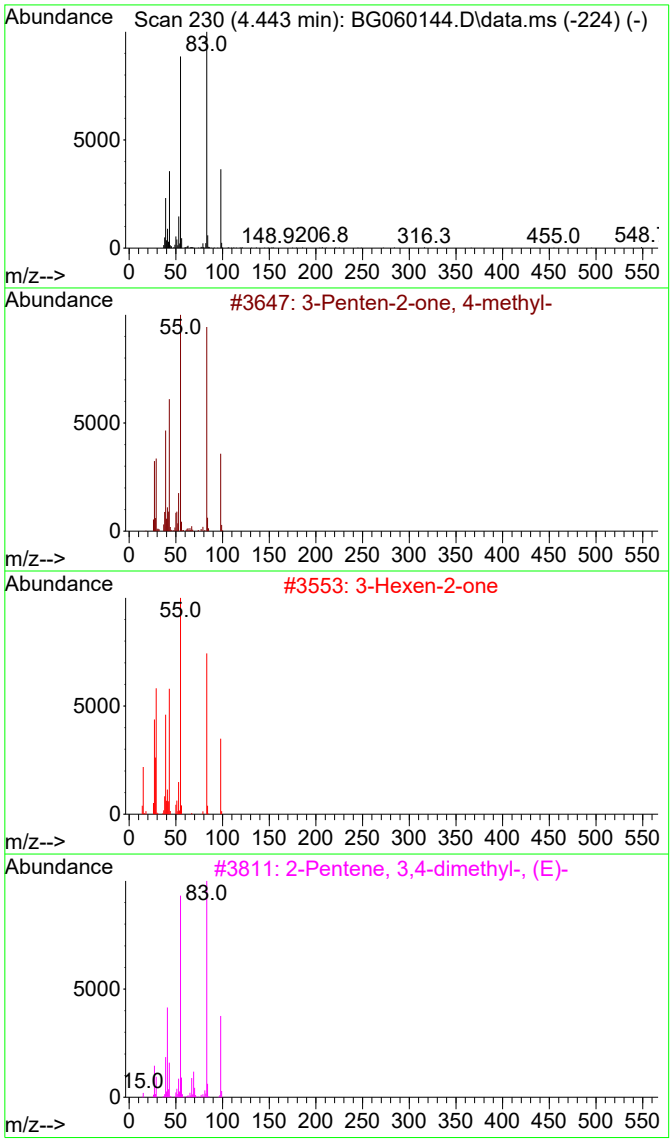
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

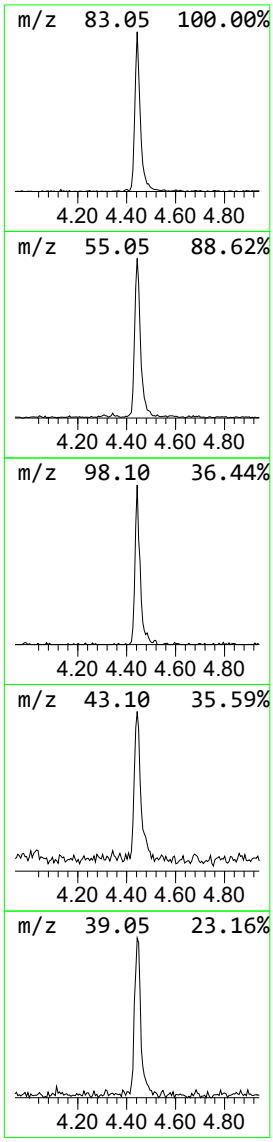
****

Peak Number 2 3-Penten-2-one, 4-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.443	11.55 ng	443730	1,4-Dichlorobenzene-d4	7.939

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	91
2	3-Hexen-2-one	98	C6H10O	000763-93-9	90
3	2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	86
4	2-Pentene, 4,4-dimethyl-, (Z)-	98	C7H14	000762-63-0	86
5	2-Pentene, 2,3-dimethyl-	98	C7H14	010574-37-5	78





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Acq On : 22 Dec 2023 18:52
Operator : MA/JU
Sample : 05897-22
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
GHL-SS-27

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG122123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

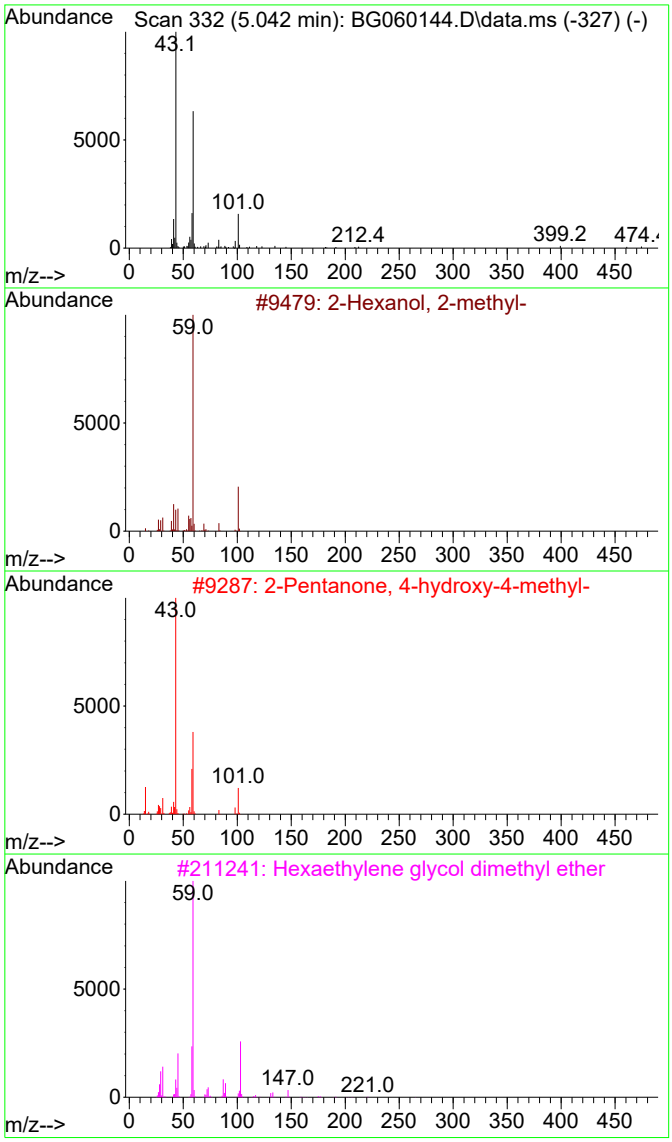
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

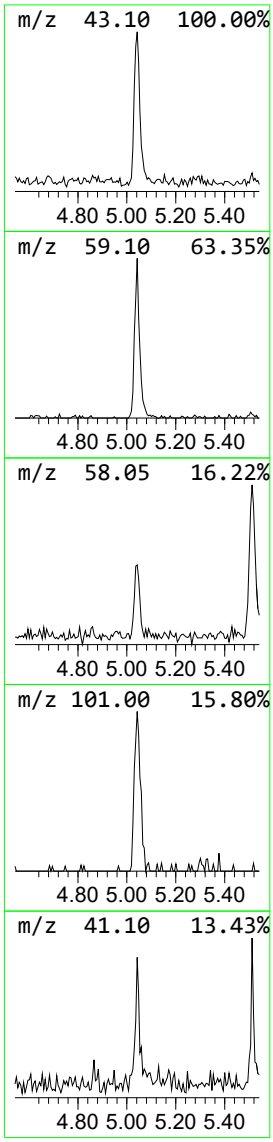
****

Peak Number 3 unknown5.042 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.042	3.22 ng	123629	1,4-Dichlorobenzene-d4	7.939

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	43
2	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	38
3	Hexaethylene glycol dimethyl ether	310	C14H30O7	001072-40-8	37
4	Tetraglyme	222	C10H22O5	000143-24-8	37
5	3-Octanol	130	C8H18O	000589-98-0	33





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Data File : BG060144.D
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Operator : MA/JU
Sample : 05897-22
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
GHL-SS-27

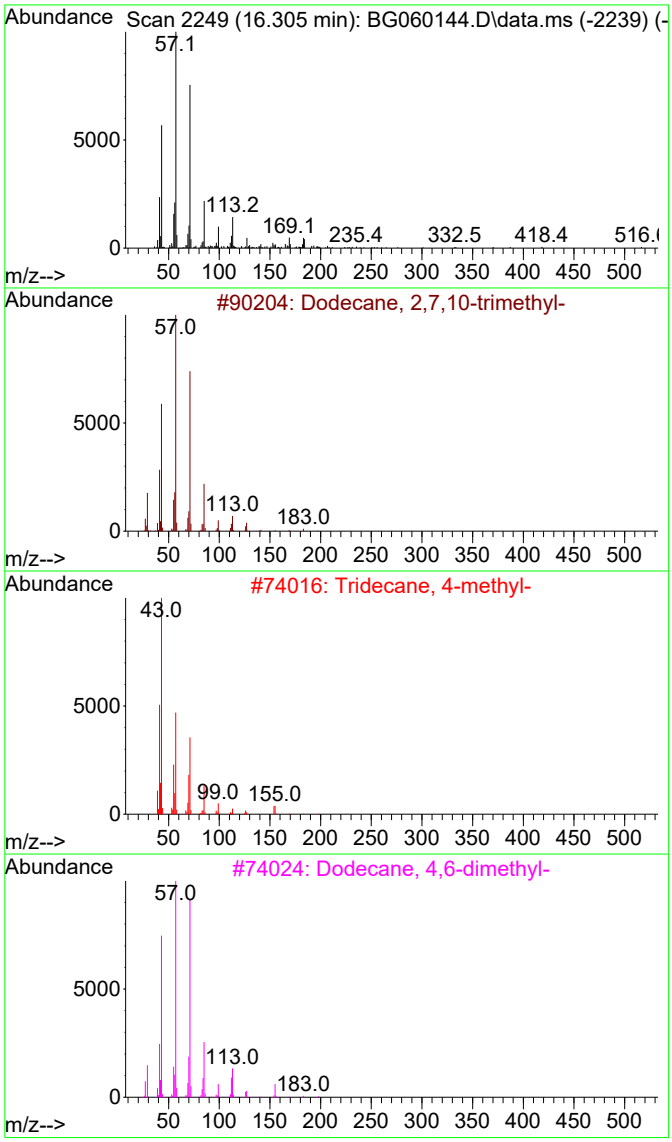
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG122123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

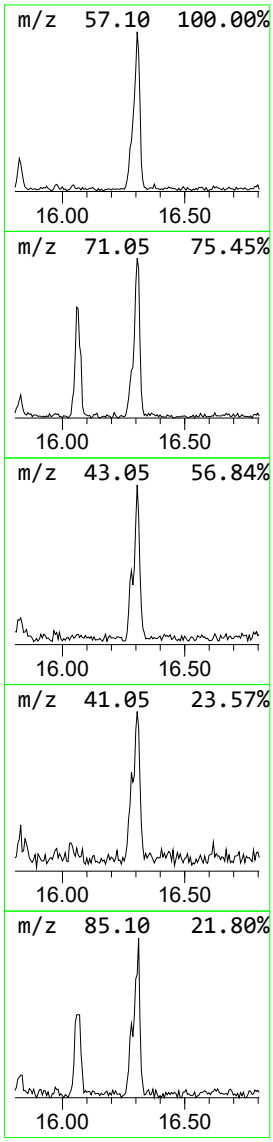
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Dodecane, 2,7,10-trimethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.305	2.10 ng	460516	Phenanthrene-d10	17.322

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dodecane, 2,7,10-trimethyl-	212	C15H32	074645-98-0	86
2	Tridecane, 4-methyl-	198	C14H30	026730-12-1	80
3	Dodecane, 4,6-dimethyl-	198	C14H30	061141-72-8	72
4	Bacchotricuneatin c	342	C20H22O5	066563-30-2	64
5	Octane, 2,6-dimethyl-	142	C10H22	002051-30-1	64





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Operator : MA/JU
Sample : 05897-22
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
GHL-SS-27

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG122123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

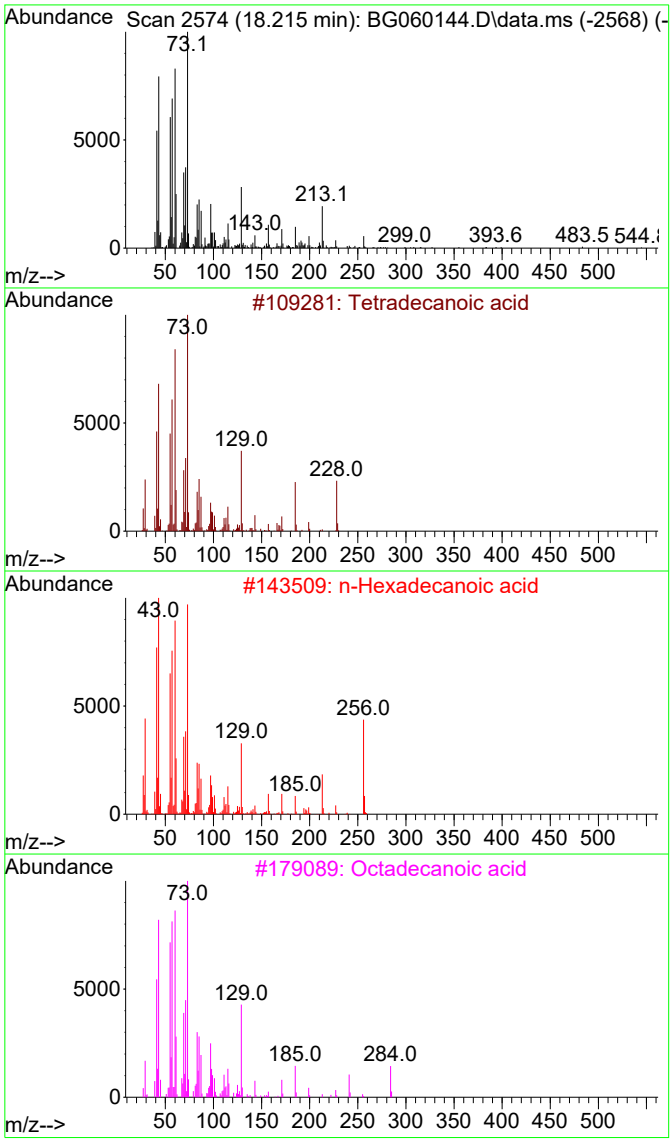
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

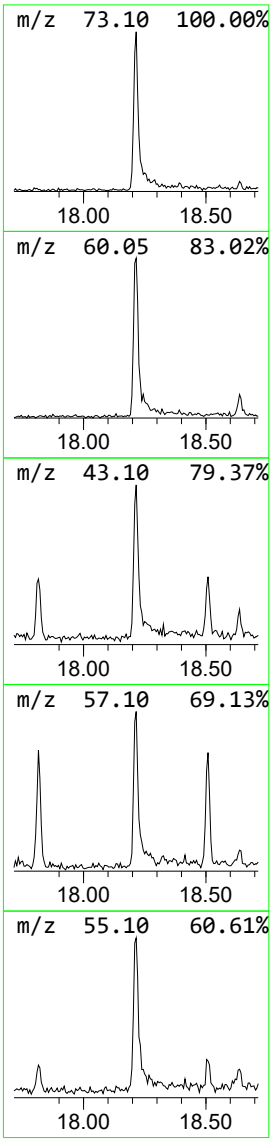
****

Peak Number 6 Tetradecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.215	3.96 ng	870094	Phenanthrene-d10	17.322

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetradecanoic acid	228	C14H28O2	000544-63-8	94
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	93
3	Octadecanoic acid	284	C18H36O2	000057-11-4	80
4	Tridecanoic acid	214	C13H26O2	000638-53-9	68
5	Pentadecanoic acid	242	C15H30O2	001002-84-2	58





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Data File : BG060144.D
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Operator : MA/JU
Sample : 05897-22
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
GHL-SS-27

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG122123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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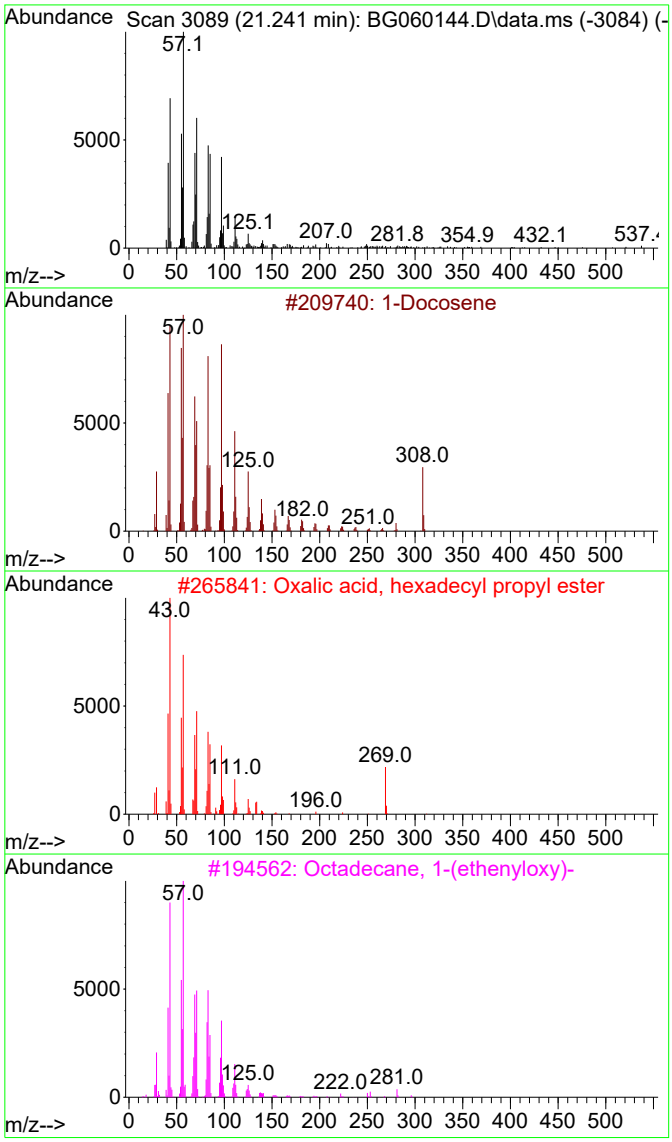
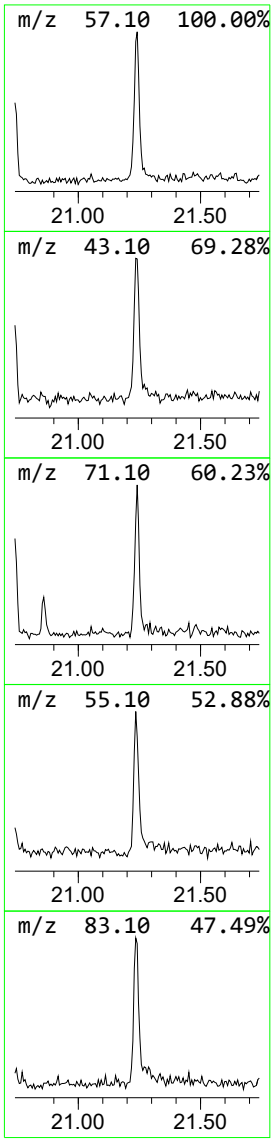
****

Peak Number 7 1-Docosene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.241	3.59 ng	667464	Chrysene-d12	21.587

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Docosene	308	C22H44	001599-67-3	93
2	Oxalic acid, hexadecyl propyl ester	356	C21H40O4	1000309-26-9	91
3	Octadecane, 1-(ethenyloxy)-	296	C20H40O	000930-02-9	90
4	Dotriacontyl pentafluoropropionate	612	C35H65F5O2	1010351-81-4	90
5	3-Eicosene, (E)-	280	C20H40	074685-33-9	84





Tentatively Identified Compound (LSC) summary

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Data File : BG060144.D
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Sample : 05897-22
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
GHL-SS-27

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG122123.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-Propanone, 1-...	3.156	7.3	ng	281536	1	7.939	768228	20.0
3-Penten-2-one,...	4.443	11.6	ng	443730	1	7.939	768228	20.0
unknown5.042	5.042	3.2	ng	123629	1	7.939	768228	20.0
Dodecane, 2,7,1...	16.305	2.1	ng	460516	4	17.322	4390190	20.0
Tetradecanoic acid	18.215	4.0	ng	870094	4	17.322	4390190	20.0
1-Docosene	21.241	3.6	ng	667464	5	21.587	3719820	20.0