LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG010224\
Data File : BG060201.D
Acq On : 2 Jan 2024 19:11
Operator : MA/JU
Sample : 05899-05
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
GHL-SS-11

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-BG122923.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG060201.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.117	3	5	10	rVB	449911	471572	3.99%	0.725%
2	4.445	226	231	242	rVB2	112081	204180	1.73%	0.314%
3	5.039	326	332	337	rBV	113644	177212	1.50%	0.272%
4	5.509	405	412	421	rBV	3187324	5003945	42.35%	7.691%
5	5.949	481	487	494	rVB3	74791	135721	1.15%	0.209%
6	7.101	674	683	698	rBV	2881739	5005849	42.37%	7.694%
7	7.935	816	825	836	rBV	730433	1297120	10.98%	1.994%
8	9.099	1015	1023	1031	rBV	1830942	3176191	26.88%	4.882%
9	10.744	1292	1303	1308	rBV	1005805	1919841	16.25%	2.951%
10	10.791	1308	1311	1319	rVB	112915	200537	1.70%	0.308%
11	12.401	1576	1585	1591	rBV2	143711	242990	2.06%	0.373%
12	12.618	1616	1622	1630	rBV2	113561	195587	1.66%	0.301%
13	13.194	1713	1720	1730	rBV	5082415	8026679	67.94%	12.337%
14	13.393	1748	1754	1760	rBV3	89195	151729	1.28%	0.233%
15	14.052	1860	1866	1871	rBV	97633	141690	1.20%	0.218%
16	14.574	1945	1955	1961	rBV	2018897	3101023	26.25%	4.766%
17	14.968	2017	2022	2029	rBV3	68930	130062	1.10%	0.200%
18	15.609	2126	2131	2137	rBV2	94246	152812	1.29%	0.235%
19	15.914	2176	2183	2190	rBV5	57184	119719	1.01%	0.184%
20	16.061	2200	2208	2219	rBV	3810867	5944579	50.31%	9.137%
21	16.302	2241	2249	2256	rVB	333364	612693	5.19%	0.942%
22	16.860	2337	2344	2349	rBV4	68011	151375	1.28%	0.233%
23	17.072	2373	2380	2384	rBV3	131864	207171	1.75%	0.318%
24	17.124	2384	2389	2401	rVB3	47278	131462	1.11%	0.202%
25	17.324	2416	2423	2428	rBV	2621495	3971755	33.62%	6.105%
26	17.812	2501	2506	2510	rBV	148306	188657	1.60%	0.290%
27	18.211	2569	2574	2578	rBV3	179262	294612	2.49%	0.453%
28	18.505	2619	2624	2629	rBV2	174385	217518	1.84%	0.334%
29	19.134	2727	2731	2738	rVB	155940	200450	1.70%	0.308%
30	19.945	2863	2869	2882	rVB	8388185	11815135	100.00%	18.160%
31	20.244	2917	2920	2925	rVB	143803	164025	1.39%	0.252%
32	20.738	3001	3004	3013	rVB	152045	204182	1.73%	0.314%
33	21.237	3083	3089	3095	rBV2	548920	895757	7.58%	1.377%
34	21.590	3142	3149	3156	rBV2	2567074	4316112	36.53%	6.634%
35	21.778	3178	3181	3190	rVB	143480	209174	1.77%	0.322%
36	22.383	3280	3284	3293	rVB2	155384	278862	2.36%	0.429%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG010224\
Data File : BG060201.D
Acq On : 2 Jan 2024 19:11
Operator : MA/JU
Sample : 05899-05
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
GHL-SS-11

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-BG122923.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	23.065	3396	3400	3408	rVB2	96056	171607	1.45%	0.264%
38	23.200	3418	3423	3428	rBV5	67945	148339	1.26%	0.228%
39	23.247	3428	3431	3437	rVB3	76137	131002	1.11%	0.201%
40	23.864	3530	3536	3541	rVB2	95330	187823	1.59%	0.289%
41	24.228	3595	3598	3606	rVB5	78728	165101	1.40%	0.254%
42	24.763	3679	3689	3705	rBV	1551032	4598486	38.92%	7.068%

Sum of corrected areas: 65060336

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG010224\
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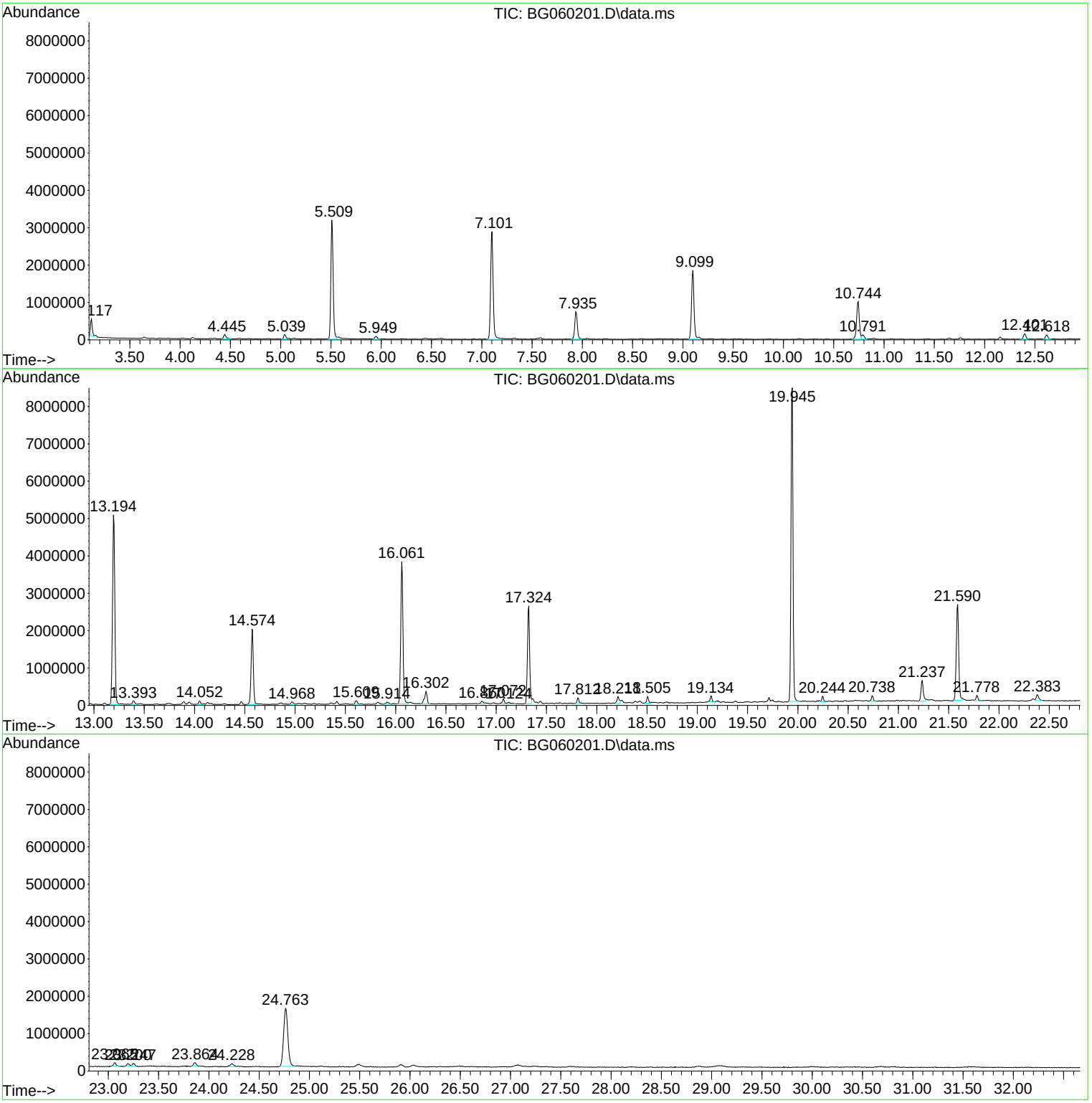
Operator : MA/JU
Sample : 05899-05
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
GHL-SS-11

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG122923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG010224\
Data File : BG060201.D
Acq On : 2 Jan 2024 19:11
Operator : MA/JU
Sample : 05899-05
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
GHL-SS-11

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG122923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

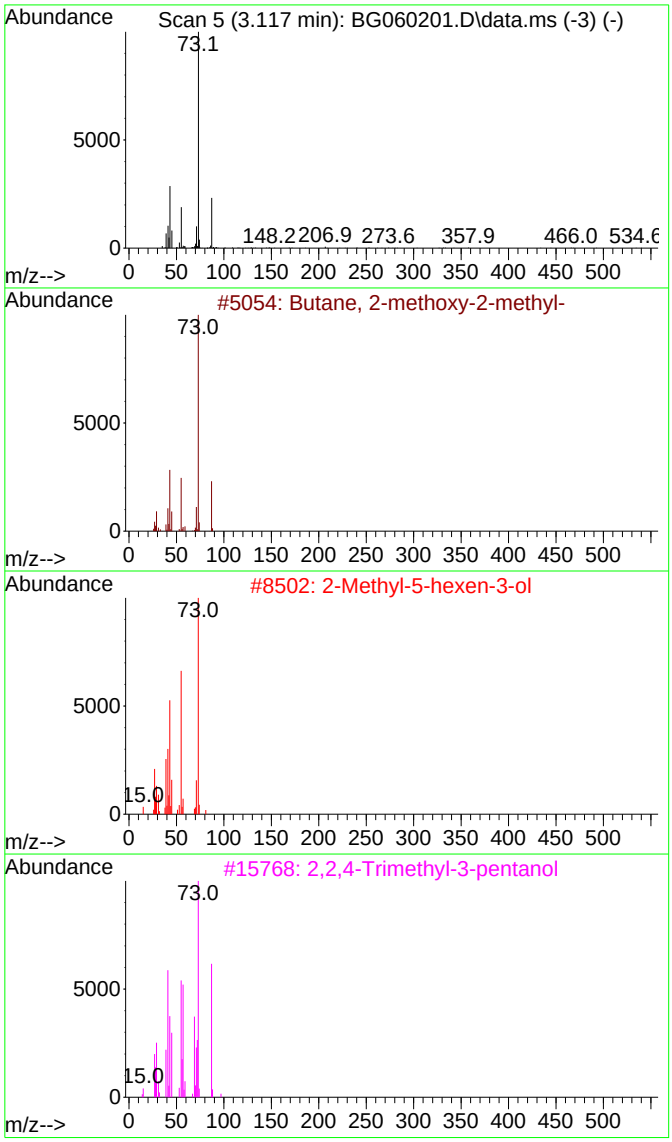
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

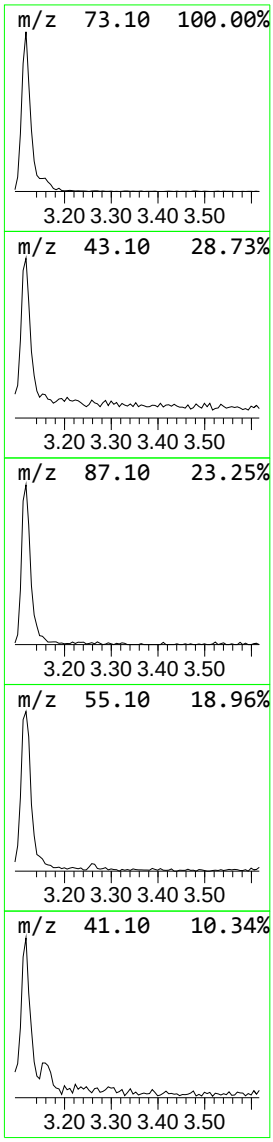
****

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.117	7.27 ng	471572	1,4-Dichlorobenzene-d4	7.935

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	64
2	2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	17
3	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	9
4	1,4-Butanediamine	88	C4H12N2	000110-60-1	9
5	1,3-Dioxolane, 2-pentadecyl-	284	C18H36O2	004360-57-0	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG010224\
Data File : BG060201.D
Acq On : 2 Jan 2024 19:11
Operator : MA/JU
Sample : 05899-05
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
GHL-SS-11

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG122923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

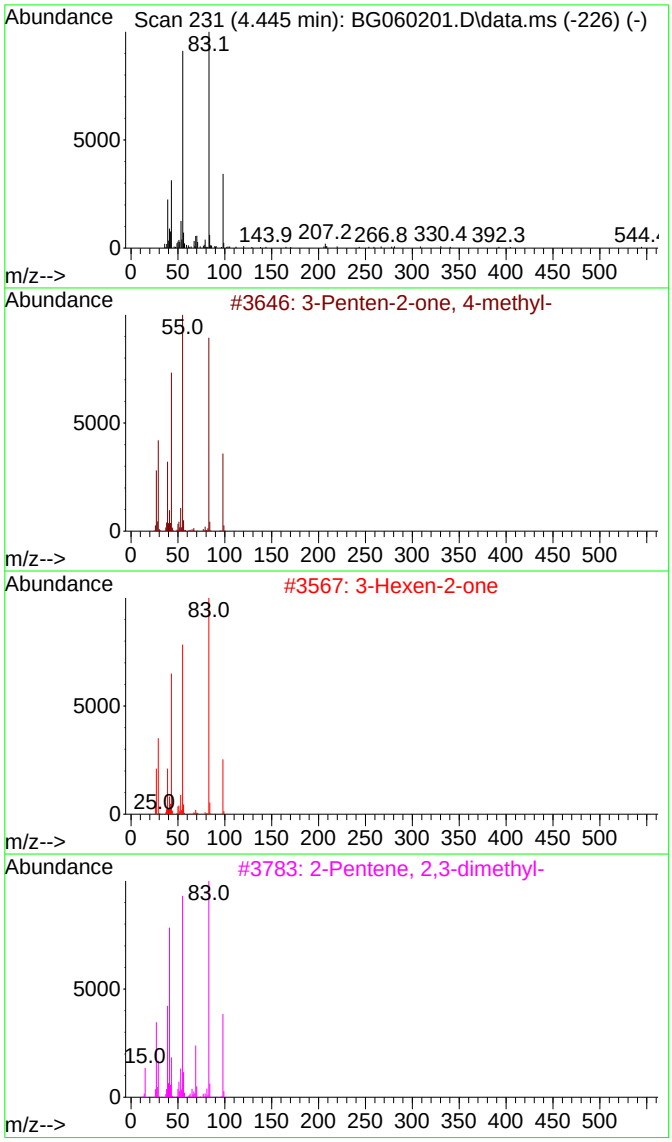
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

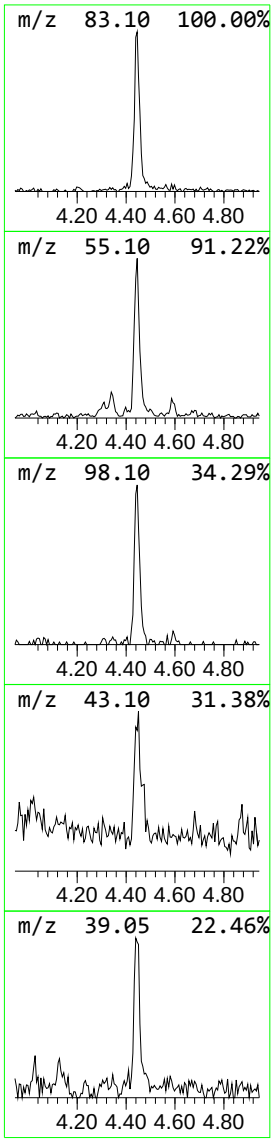
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.445	3.15 ng	204180	1,4-Dichlorobenzene-d4	7.935

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





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG010224\
Data File : BG060201.D
Acq On : 2 Jan 2024 19:11
Operator : MA/JU
Sample : 05899-05
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
GHL-SS-11

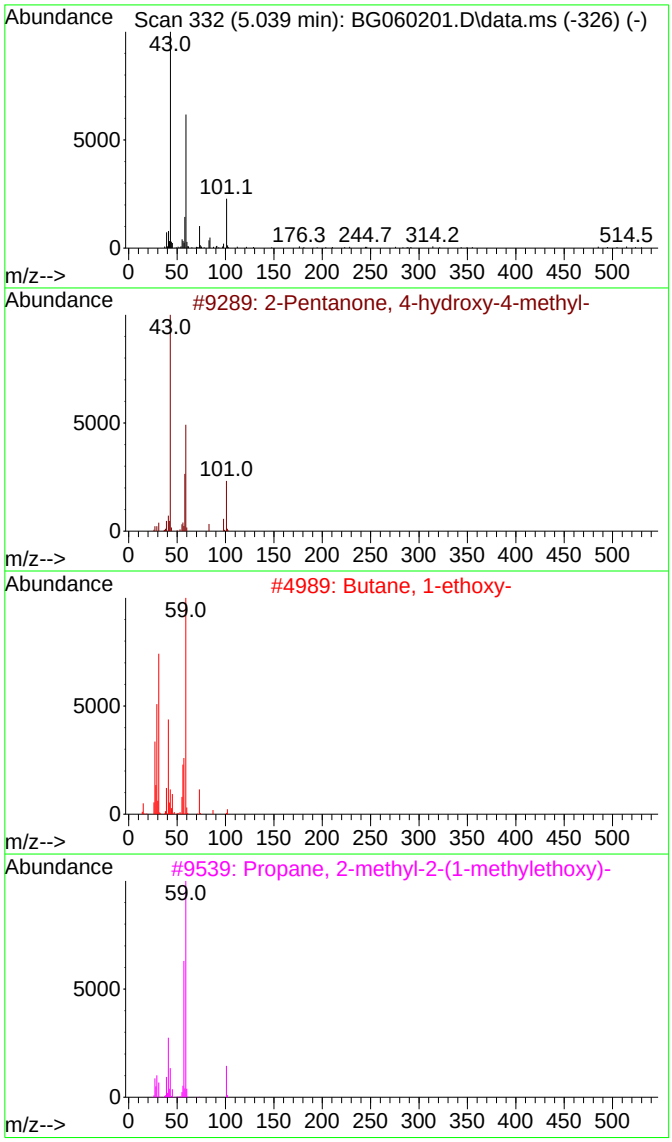
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG122923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

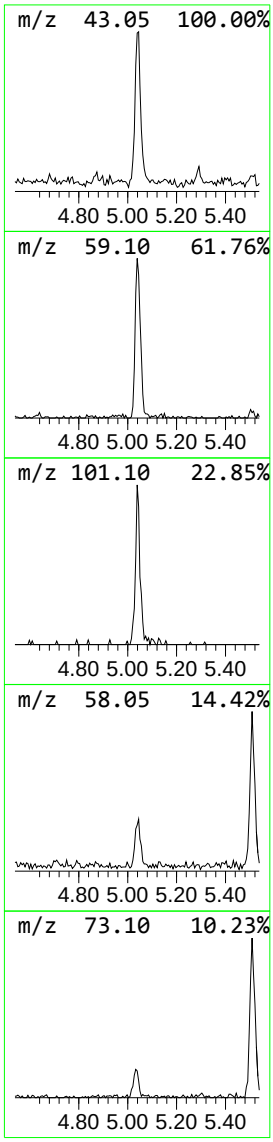
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.039	2.73 ng	177212	1,4-Dichlorobenzene-d4	7.935

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	43
3	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	40
4	Methyl 2,5,8,11,14,17-hexaoxanon...	324	C14H28O8	1000366-81-4	25
5	Guanidine	59	CH5N3	000113-00-8	25





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG010224\
Data File : BG060201.D
Acq On : 2 Jan 2024 19:11
Operator : MA/JU
Sample : 05899-05
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
GHL-SS-11

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG122923.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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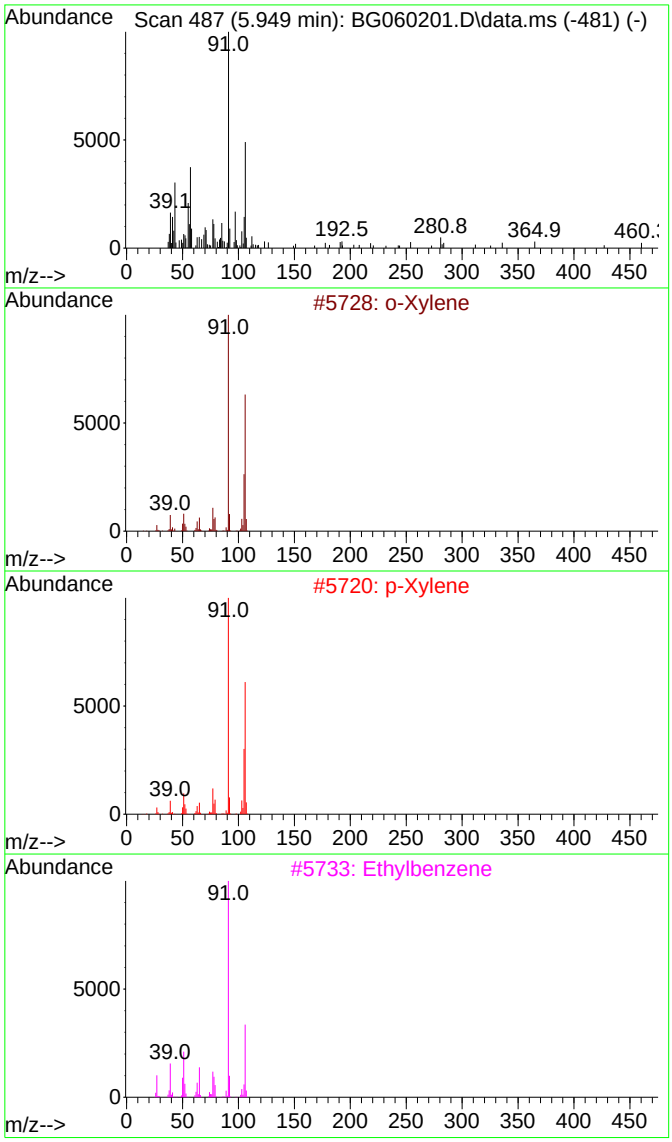
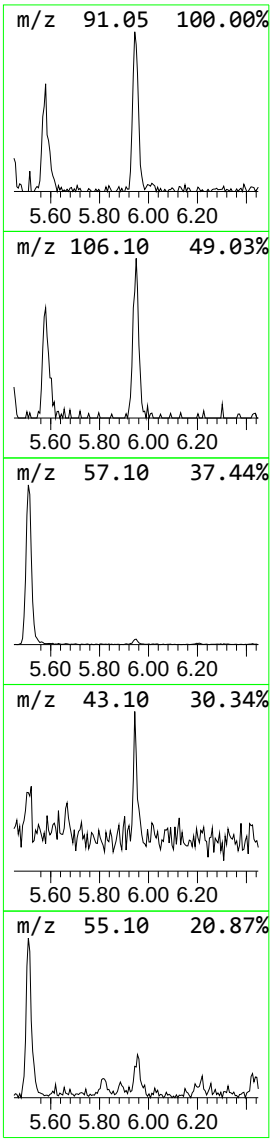
Peak Number 4 o-Xylene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.949	2.09 ng	135721	1,4-Dichlorobenzene-d4	7.935

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	o-Xylene	106	C8H10	000095-47-6	53
2	p-Xylene	106	C8H10	000106-42-3	53
3	Ethylbenzene	106	C8H10	000100-41-4	53
4	1,3-Cyclopentadiene, 5-(1-methyl...	106	C8H10	002175-91-9	49
5	Benzene, 1,3-dimethyl-	106	C8H10	000108-38-3	47





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG010224\
Data File : BG060201.D
Acq On : 2 Jan 2024 19:11
Operator : MA/JU
Sample : 05899-05
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
GHL-SS-11

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG122923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

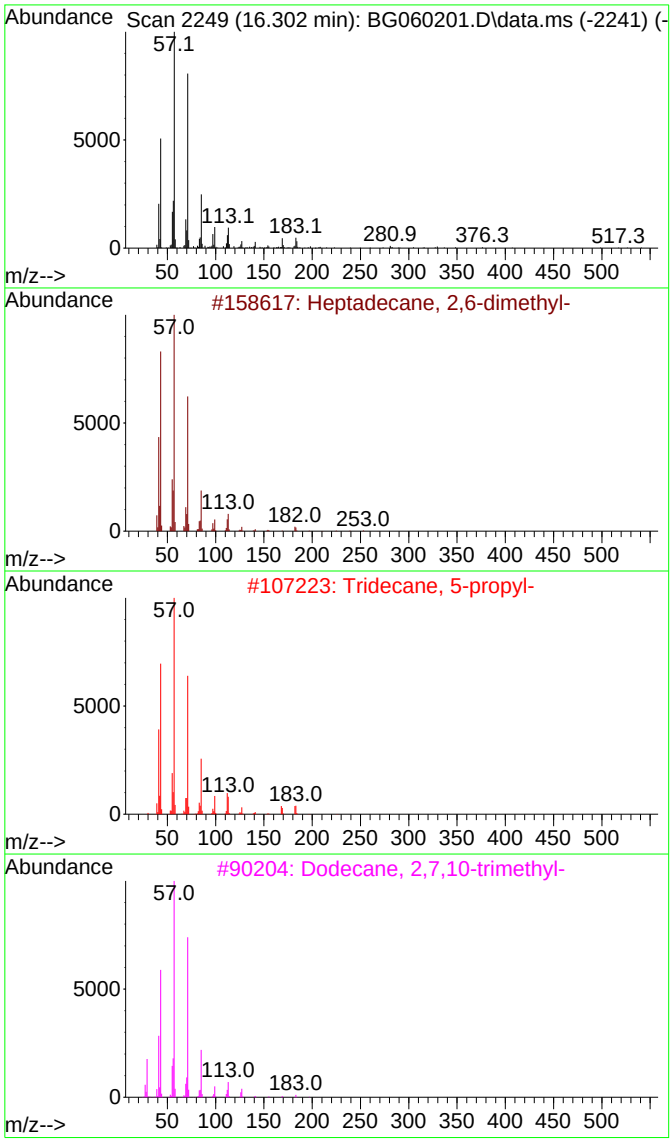
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

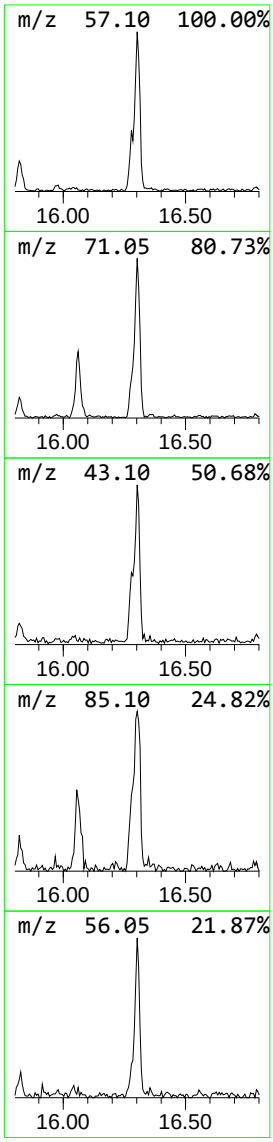
****

Peak Number 7 Heptadecane, 2,6-dimethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.302	3.09 ng	612693	Phenanthrene-d10	17.324

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane, 2,6-dimethyl-	268	C19H40	054105-67-8	90
2	Tridecane, 5-propyl-	226	C16H34	055045-11-9	86
3	Dodecane, 2,7,10-trimethyl-	212	C15H32	074645-98-0	86
4	Heptadecane, 2,6,10,14-tetramethyl-	296	C21H44	018344-37-1	83
5	Dodecane, 2,6,11-trimethyl-	212	C15H32	031295-56-4	78





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG010224\
Data File : BG060201.D
Acq On : 2 Jan 2024 19:11
Operator : MA/JU
Sample : 05899-05
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
GHL-SS-11

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG122923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

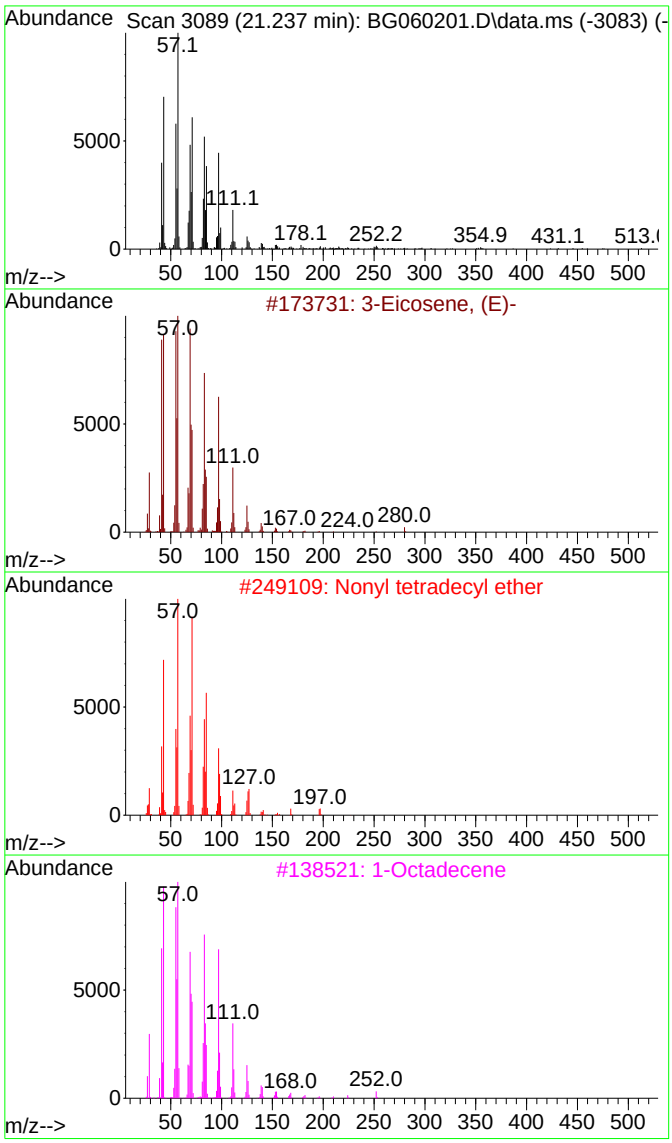
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

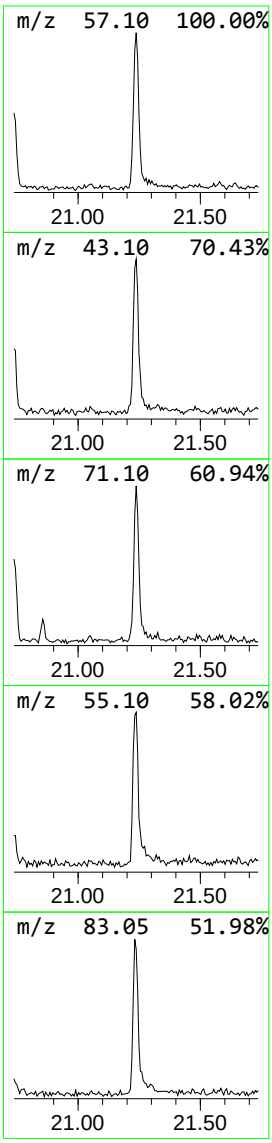
****

Peak Number 8 3-Eicosene, (E)- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.237	4.15 ng	895757	Chrysene-d12	21.590

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Eicosene, (E)-	280	C20H40	074685-33-9	89
2	Nonyl tetradecyl ether	340	C23H48O	1000406-37-6	64
3	1-Octadecene	252	C18H36	000112-88-9	64
4	Cyclotetradecane	196	C14H28	000295-17-0	64
5	Carbonic acid, eicosyl vinyl ester	368	C23H44O3	1000382-54-3	52





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG010224\
Data File : BG060201.D
Acq On : 2 Jan 2024 19:11
Operator : MA/JU
Sample : 05899-05
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
GHL-SS-11

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG122923.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
Butane, 2-metho...	3.117	7.3	ng	471572	1	7.935	1297120	20.0
3-Penten-2-one,...	4.445	3.1	ng	204180	1	7.935	1297120	20.0
2-Pentanone, 4-...	5.039	2.7	ng	177212	1	7.935	1297120	20.0
o-Xylene	5.949	2.1	ng	135721	1	7.935	1297120	20.0
Heptadecane, 2,...	16.302	3.1	ng	612693	4	17.324	3971760	20.0
3-Eicosene, (E)-	21.237	4.2	ng	895757	5	21.590	4316110	20.0