LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG030519\
Data File : BG039773.D
Acq On : 5 Mar 2019 20:45
Operator : JU/SJ
Sample : K1727-06
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MW-6

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-BG030419.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.210	16	21	29	rBV	163460	292519	7.10%	1.603%
2	3.281	29	33	44	rVB	137025	197276	4.79%	1.081%
3	5.701	437	445	457	rBV	381574	620669	15.07%	3.402%
4	7.299	710	717	727	rBV	263843	463544	11.25%	2.541%
5	7.681	775	782	794	rVB	706947	1232673	29.93%	6.756%
6	8.156	856	863	872	rBV	151403	262938	6.38%	1.441%
7	8.479	910	918	929	rBV	579184	988440	24.00%	5.418%
8	9.331	1055	1063	1075	rBV	562635	1031053	25.03%	5.651%
9	10.976	1335	1343	1351	rBV	217620	398169	9.67%	2.182%
10	13.402	1747	1756	1764	rBV	1566637	2474527	60.08%	13.563%
11	14.783	1984	1991	2000	rVB2	390390	631542	15.33%	3.462%
12	16.269	2237	2244	2256	rBV	1403856	2140297	51.97%	11.731%
13	17.526	2451	2458	2464	rBV	559519	822408	19.97%	4.508%
14	18.372	2596	2602	2608	rBV2	45494	67058	1.63%	0.368%
15	20.123	2892	2900	2911	rBV	2927203	4118700	100.00%	22.575%
16	21.403	3113	3118	3124	rBV2	39332	71719	1.74%	0.393%
17	21.814	3181	3188	3197	rVB	569584	936823	22.75%	5.135%
18	21.961	3208	3213	3219	rVB	29468	41982	1.02%	0.230%
19	22.590	3314	3320	3325	rBV2	40231	70611	1.71%	0.387%
20	23.306	3436	3442	3449	rVB3	49729	99088	2.41%	0.543%
21	24.141	3578	3584	3593	rVB2	50203	112926	2.74%	0.619%
22	25.192	3743	3763	3780	rVB	304081	1026135	24.91%	5.624%
23	26.308	3944	3953	3963	rVB4	30072	95907	2.33%	0.526%
24	27.724	4188	4194	4205	rVB7	14283	47419	1.15%	0.260%

Sum of corrected areas: 18244423

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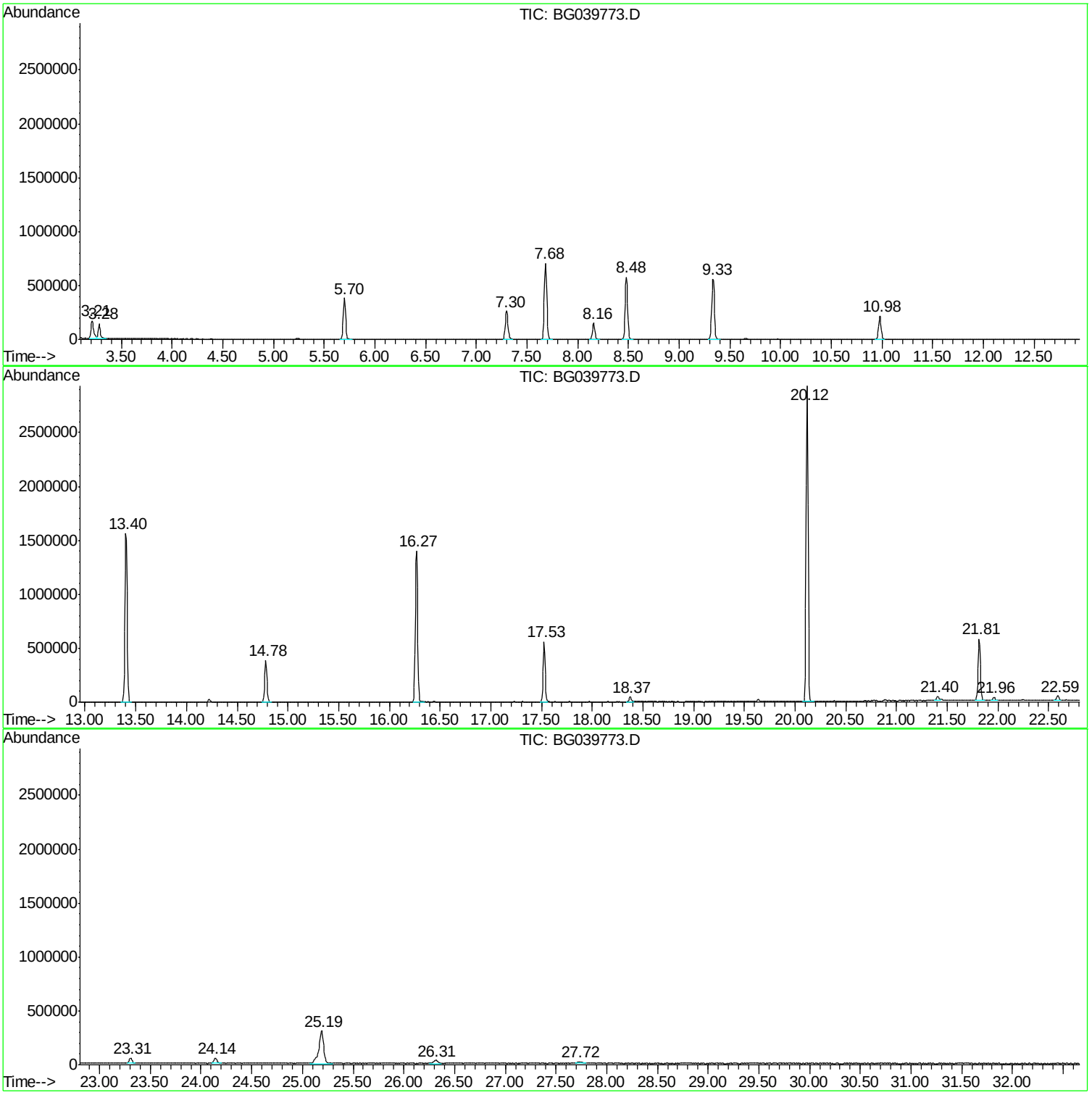
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW-6

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG030419.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P



Library Search Compound Report

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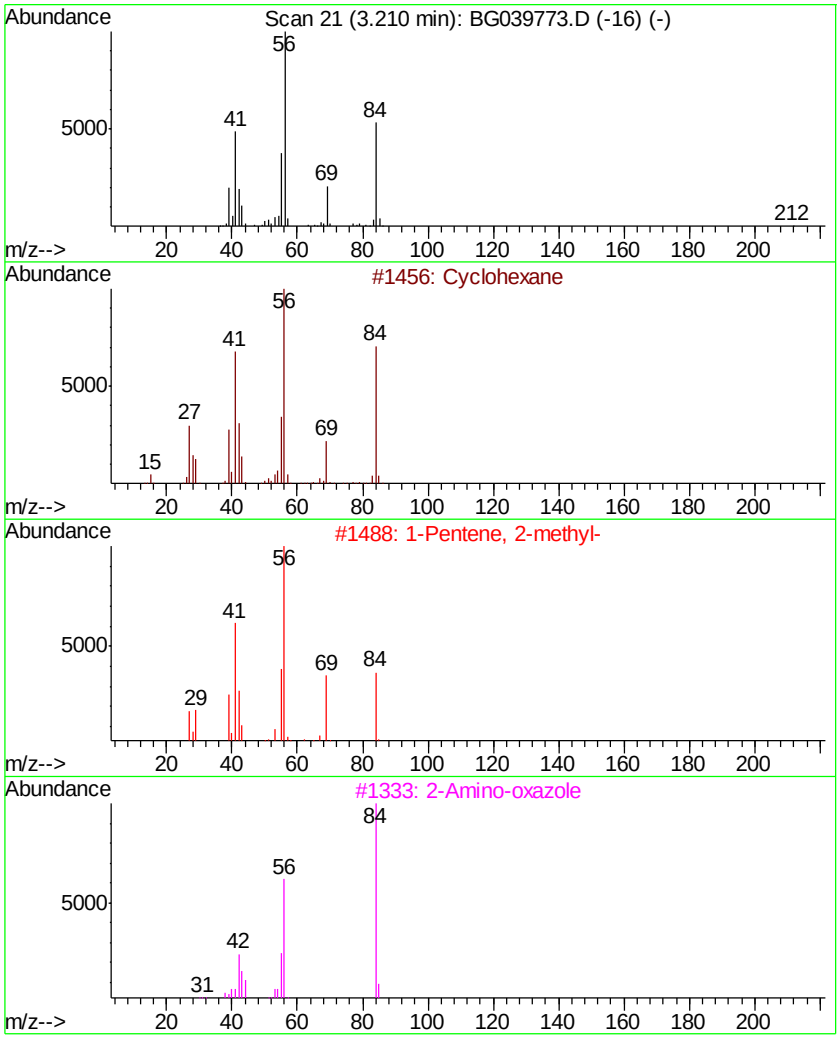
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

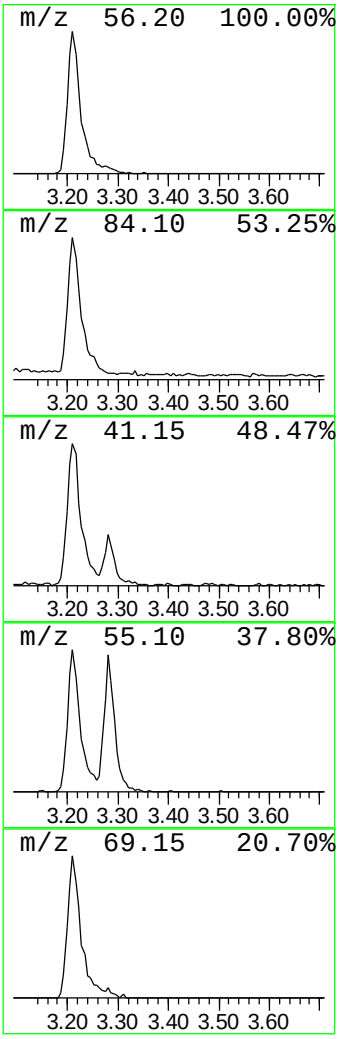
****

Peak Number 1 1-Pentene, 2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.21	22.25 ng	292519	1,4-Dichlorobenzene-d4	8.16

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexane	84	C6H12	000110-82-7	91
2	1-Pentene, 2-methyl-	84	C6H12	000763-29-1	78
3	2-Amino-oxazole	84	C3H4N2O	004570-45-0	45
4	Cyclopentane, methyl-	84	C6H12	000096-37-7	45
5	Cyclobutanone, 2-methyl-	84	C5H8O	001517-15-3	45





Library Search Compound Report

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Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MW-6

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG030419.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

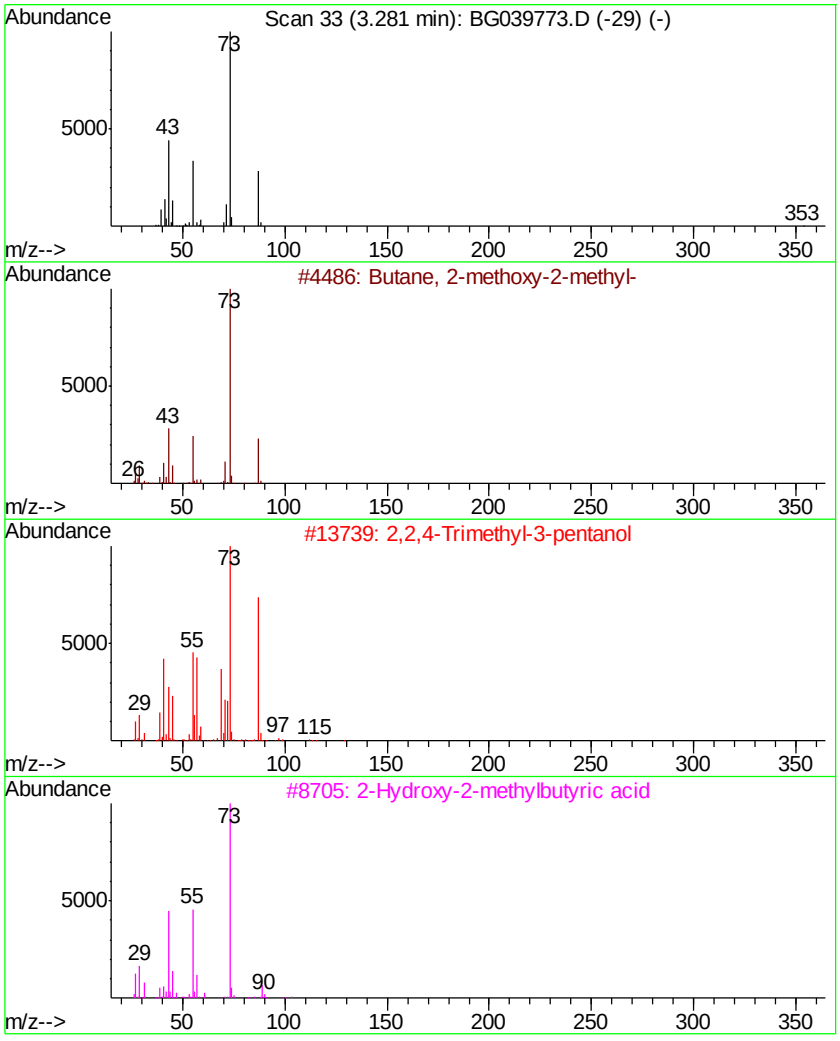
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

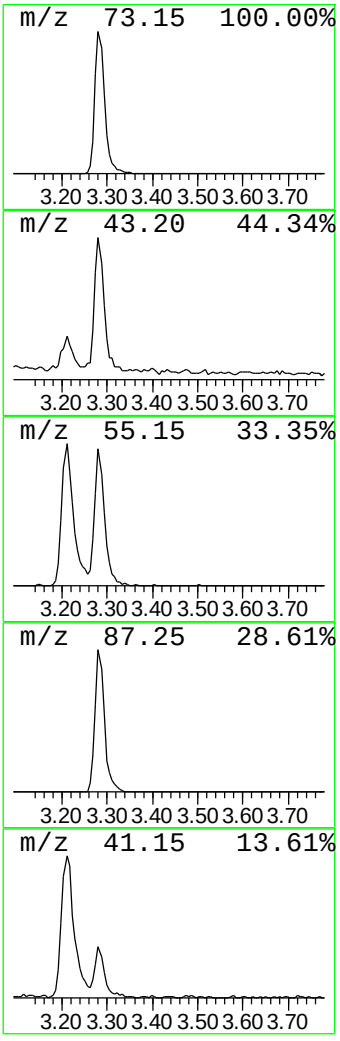
****

Peak Number 2 Butane, 2-methoxy-2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.28	15.01 ng	197276	1,4-Dichlorobenzene-d4	8.16

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3	2-Hydroxy-2-methylbutyric acid	118	C5H10O3	003739-30-8	25
4	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12
5	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	9





Library Search Compound Report

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Data File : BG039773.D
Acq On : 5 Mar 2019 20:45
Operator : JU/SJ
Sample : K1727-06
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MW-6

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG030419.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
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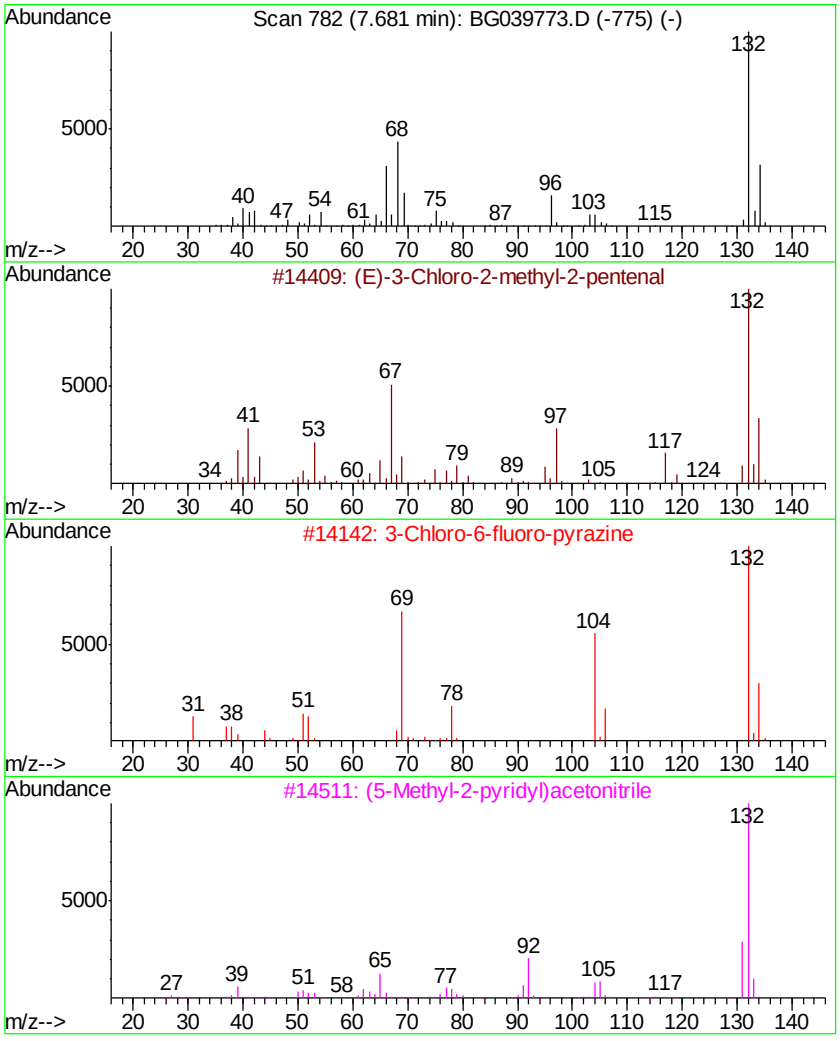
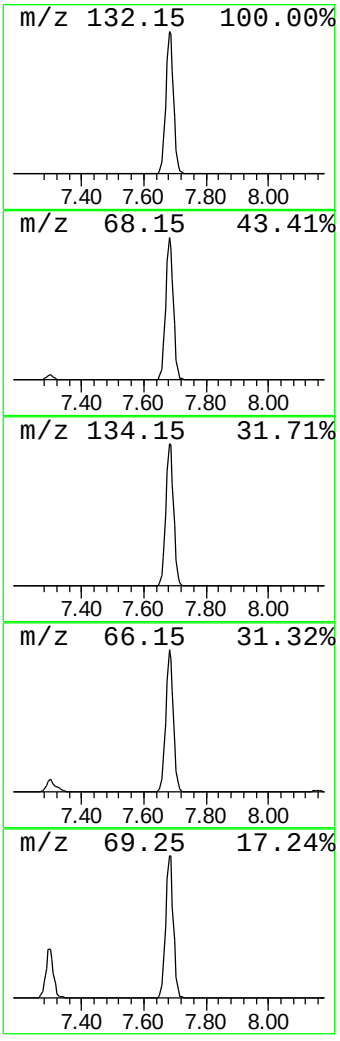
****

Peak Number 3 unknown7.68 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.68	93.76 ng	1232670	1,4-Dichlorobenzene-d4	8.16

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	27
2	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
3	(5-Methyl-2-pyridyl)acetonitrile	132	C8H8N2	1000241-93-9	10
4	5-Aminoindole	132	C8H8N2	005192-03-0	10
5	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9





Library Search Compound Report

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ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MW-6

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG030419.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
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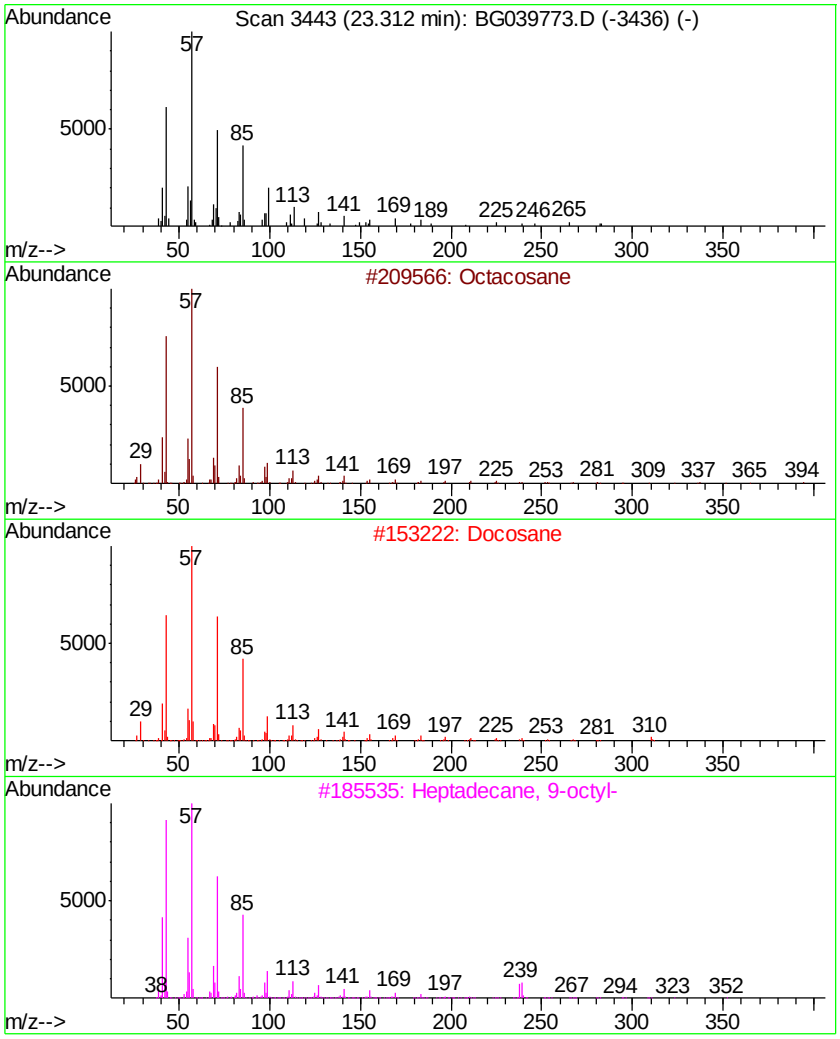
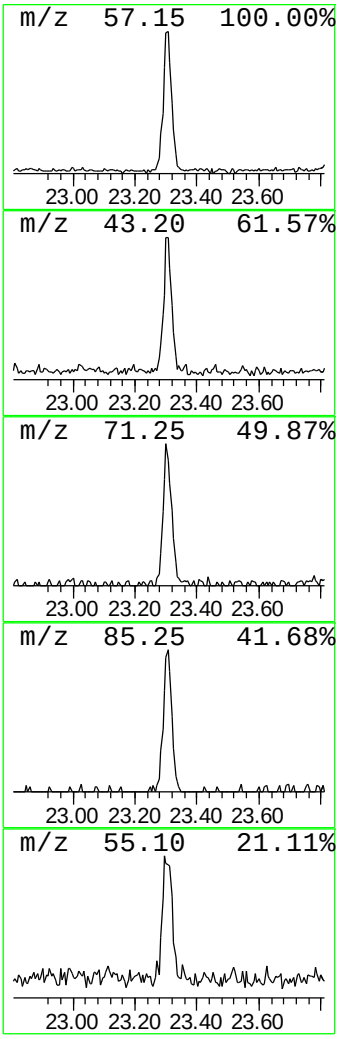
****

Peak Number 5 Octacosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.31	2.12 ng	99088	Chrysene-d12	21.81

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane	394	C28H58	000630-02-4	90
2	Docosane	310	C22H46	000629-97-0	90
3	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	87
4	Tetracosane	338	C24H50	000646-31-1	87
5	Heneicosane	296	C21H44	000629-94-7	87





Library Search Compound Report

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Sample : K1727-06
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MW-6

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG030419.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
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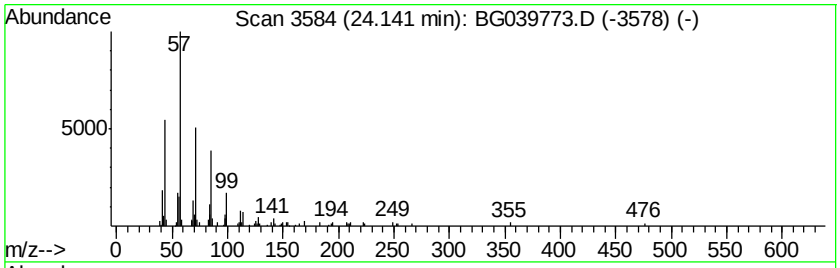
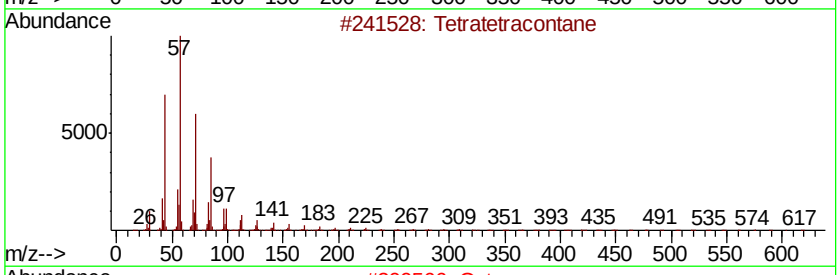
****

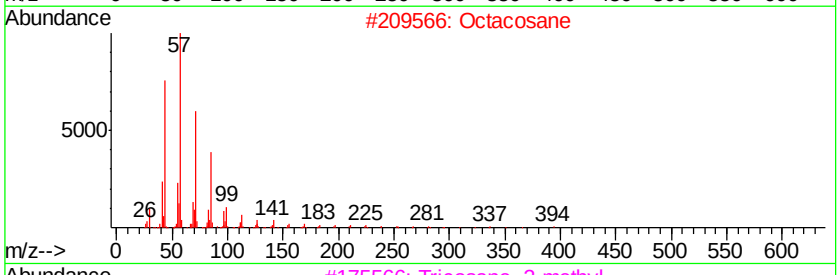
Peak Number 6 Tetratetracontane Concentration Rank 5

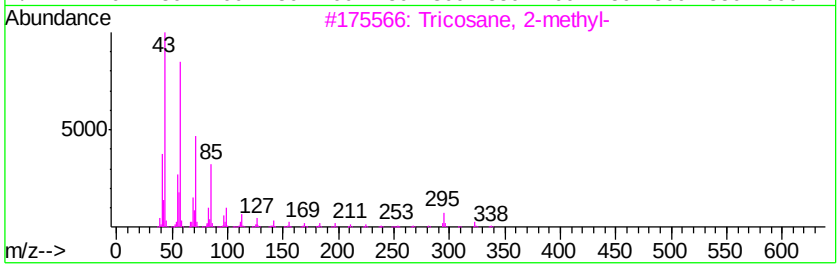
R.T.	EstConc	Area	Relative to ISTD	R.T.
24.14	2.20 ng	112926	Perylene-d12	25.19

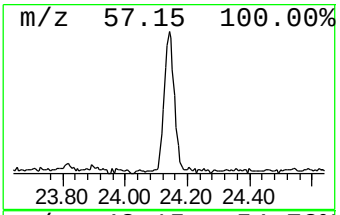
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetratetracontane	619	C44H90	007098-22-8	83
2	Octacosane	394	C28H58	000630-02-4	81
3	Tricosane, 2-methyl-	338	C24H50	001928-30-9	80
4	Eicosane	282	C20H42	000112-95-8	80
5	Heptadecane	240	C17H36	000629-78-7	80

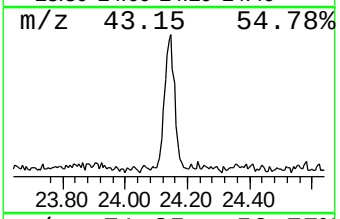


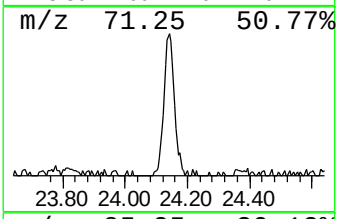


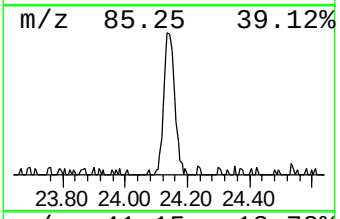


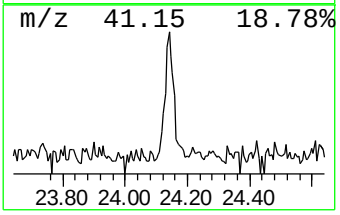












Tentatively Identified Compound (LSC) summary

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ClientSampleId : MW-6

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
1-Pentene, 2-methyl-	3.21	22.3	ng	292519	1	8.16	262938	20.0
Butane, 2-methoxy...	3.28	15.0	ng	197276	1	8.16	262938	20.0
unknown7.68	7.68	93.8	ng	1232670	1	8.16	262938	20.0
Octacosane	23.31	2.1	ng	99088	5	21.81	936823	20.0
Tetratetracontane	24.14	2.2	ng	112926	6	25.19	1026140	20.0