LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG103119\
Data File : BG043443.D
Acq On : 31 Oct 2019 20:59
Operator : JU
Sample : K5615-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : RBR-29

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-BG102119.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	3.196	13	18	32	rVB	72989	150744	4.35%	0.828%
2	5.129	340	347	358	rBV	135627	219850	6.34%	1.207%
3	5.611	422	429	442	rBV	678778	1182728	34.12%	6.496%
4	7.209	693	701	713	rBV	714138	1314120	37.91%	7.217%
5	7.568	752	762	772	rBV	742396	1330279	38.38%	7.306%
6	8.026	832	840	848	rBV	150410	267426	7.72%	1.469%
7	8.349	886	895	905	rBV	570922	1020673	29.45%	5.606%
8	9.183	1029	1037	1047	rBV	381820	762547	22.00%	4.188%
9	10.828	1309	1317	1329	rBV	162963	341684	9.86%	1.877%
10	13.273	1725	1733	1748	rBV	1231055	2009822	57.98%	11.038%
11	14.101	1868	1874	1884	rBV	48547	90967	2.62%	0.500%
12	14.648	1960	1967	1974	rBV	307662	504043	14.54%	2.768%
13	14.712	1974	1978	1988	rVB2	28863	49410	1.43%	0.271%
14	16.140	2213	2221	2235	rBV	1075108	1829634	52.79%	10.049%
15	17.397	2428	2435	2439	rBV	364050	593431	17.12%	3.259%
16	17.438	2439	2442	2451	rVV	64685	113089	3.26%	0.621%
17	18.284	2579	2586	2592	rBV5	36067	72562	2.09%	0.399%
18	19.448	2778	2784	2790	rBV	59230	92959	2.68%	0.511%
19	19.806	2842	2845	2852	rVB	46206	73933	2.13%	0.406%
20	20.006	2872	2879	2892	rBV	2482231	3466180	100.00%	19.037%
21	20.799	3009	3014	3023	rBV2	28232	43385	1.25%	0.238%
22	21.299	3095	3099	3110	rBV2	117131	251779	7.26%	1.383%
23	21.663	3152	3161	3173	rBV	425018	834193	24.07%	4.582%
24	21.851	3188	3193	3200	rBV	42529	64028	1.85%	0.352%
25	22.009	3206	3220	3225	rBV	55729	220256	6.35%	1.210%
26	22.450	3290	3295	3302	rBV2	47566	84480	2.44%	0.464%
27	23.138	3406	3412	3421	rVB2	50065	97949	2.83%	0.538%
28	23.331	3438	3445	3453	rVB3	37544	78290	2.26%	0.430%
29	23.937	3542	3548	3555	rVB4	39525	86245	2.49%	0.474%
30	24.865	3695	3706	3720	rBV	296421	902372	26.03%	4.956%
31	25.993	3890	3898	3905	rBV6	23590	58791	1.70%	0.323%

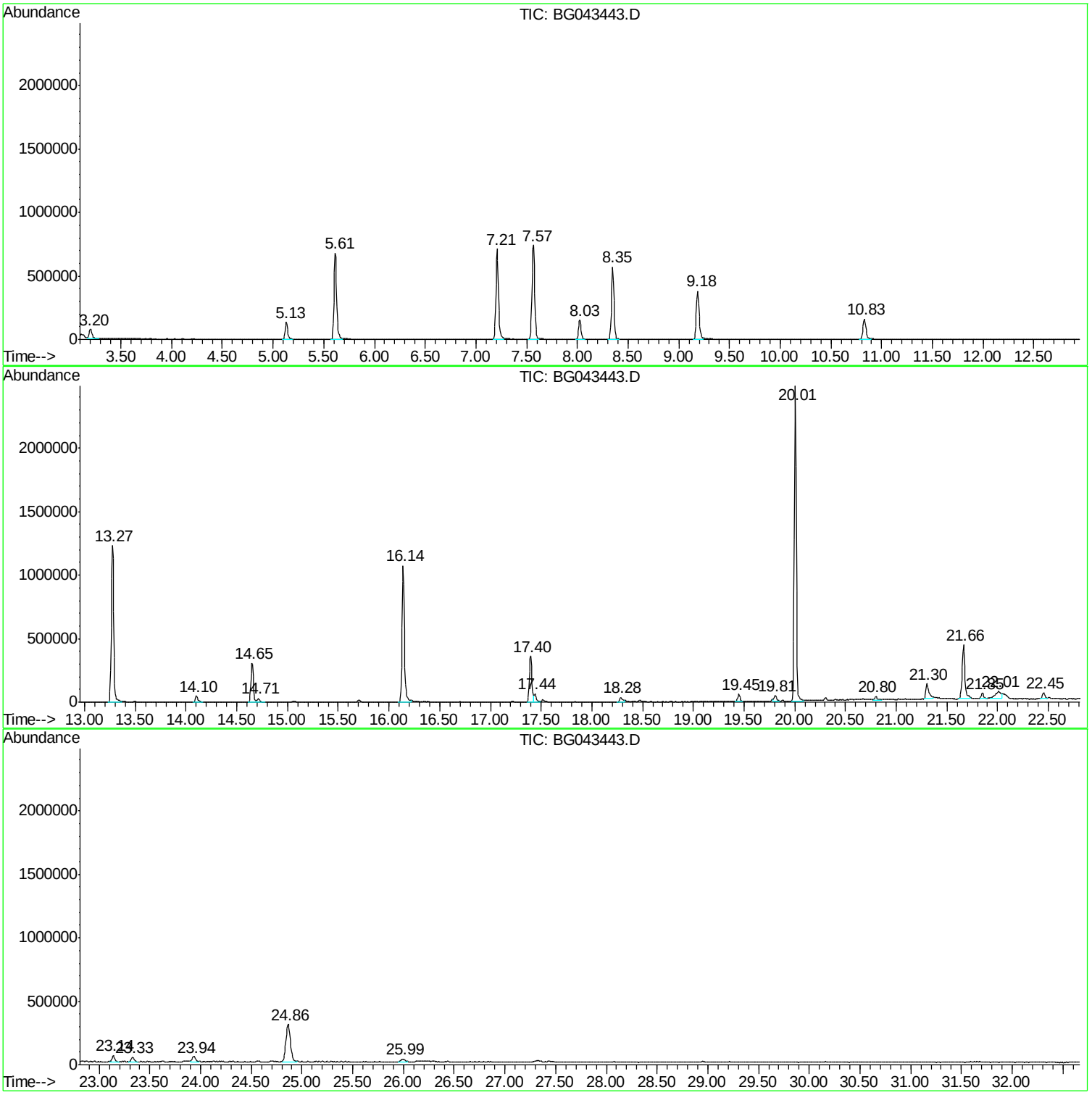
Sum of corrected areas: 18207849

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG103119\
Data File : BG043443.D
Acq On : 31 Oct 2019 20:59
Operator : JU
Sample : K5615-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
RBR-29

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG102119.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

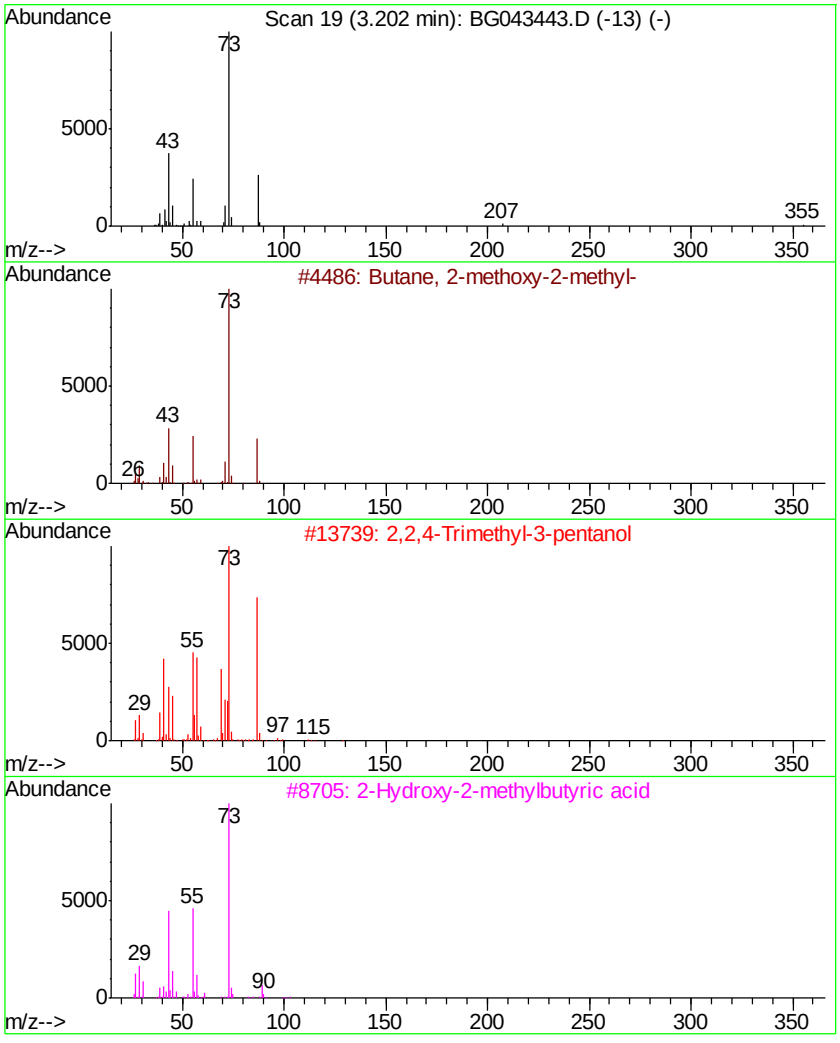
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

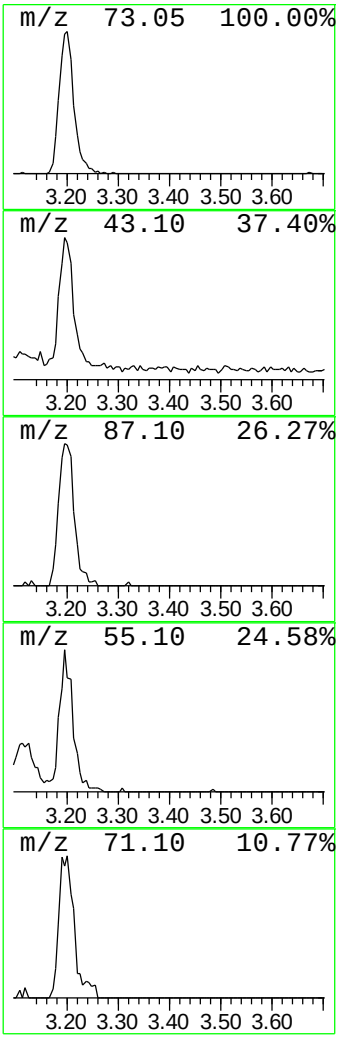
****

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.20	11.27 ng	150744	1,4-Dichlorobenzene-d4	8.03

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3	2-Hydroxy-2-methylbutyric acid	118	C5H10O3	003739-30-8	25
4	N-Ethylformamide	73	C3H7NO	000627-45-2	9
5	Silane, tetramethyl-	88	C4H12Si	000075-76-3	9





Library Search Compound Report

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Data File : BG043443.D
Acq On : 31 Oct 2019 20:59
Operator : JU
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Misc :
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Instrument : BNA_G
ClientSampleId : RBR-29

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG102119.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

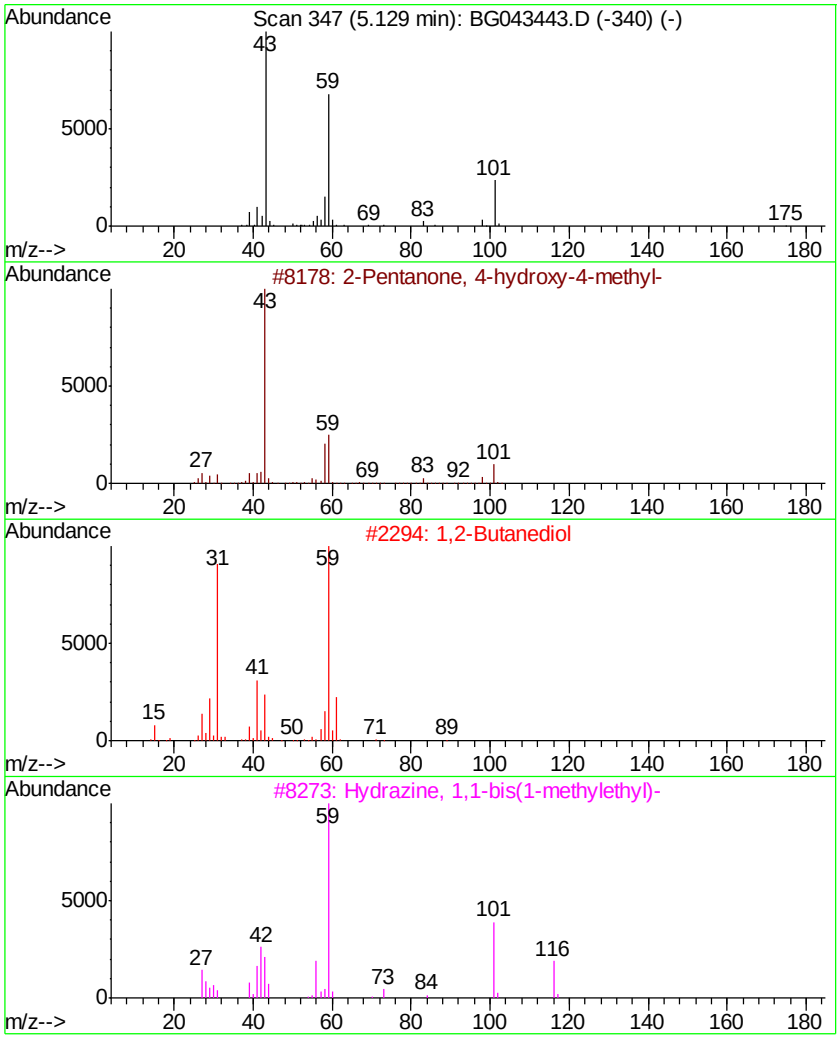
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

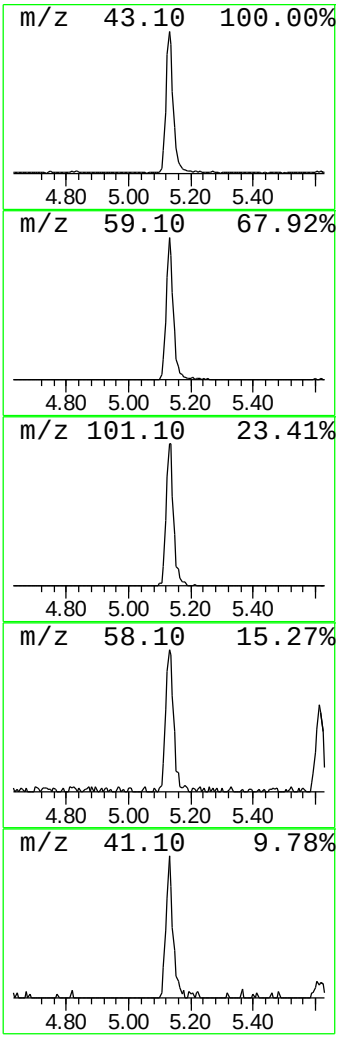
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.13	16.44 ng	219850	1,4-Dichlorobenzene-d4	8.03

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2	1,2-Butanediol	90	C4H10O2	000584-03-2	37
3	Hydrazine, 1,1-bis(1-methylethyl)-	116	C6H16N2	000921-14-2	28
4	Methyl 2,5,8,11-tetraoxatridecan...	236	C10H20O6	1000366-78-2	23
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9





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Instrument : BNA_G
ClientSampleId : RBR-29

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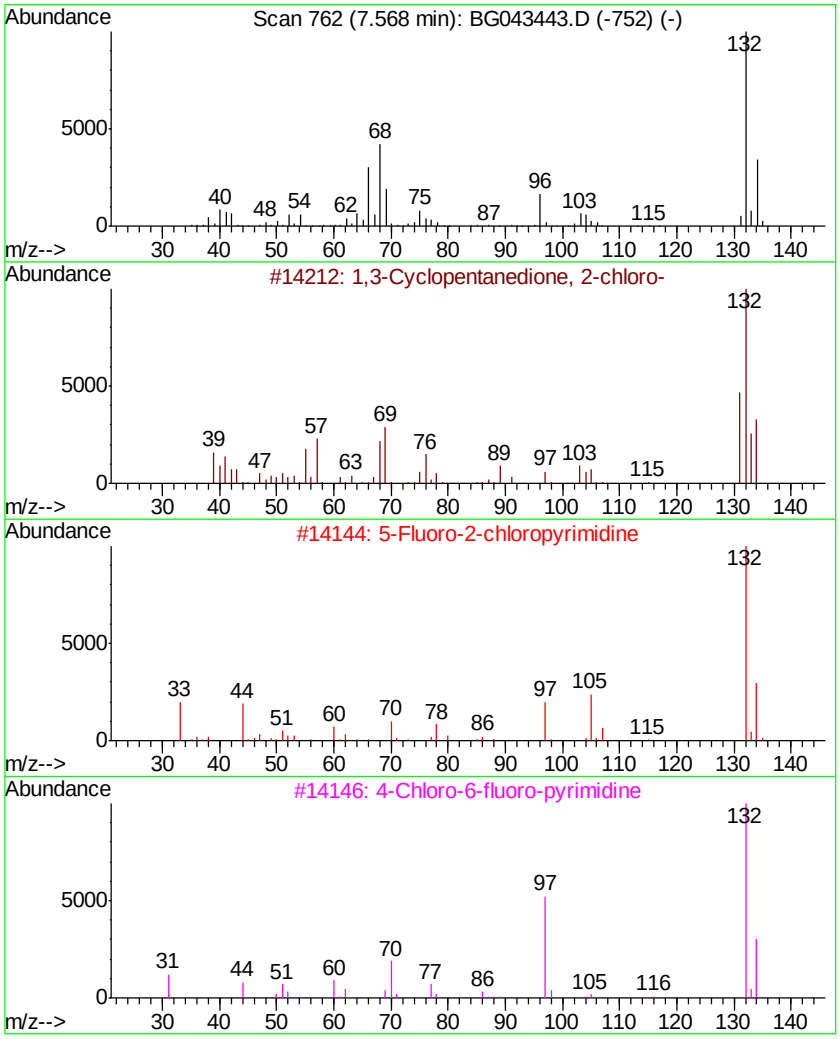
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

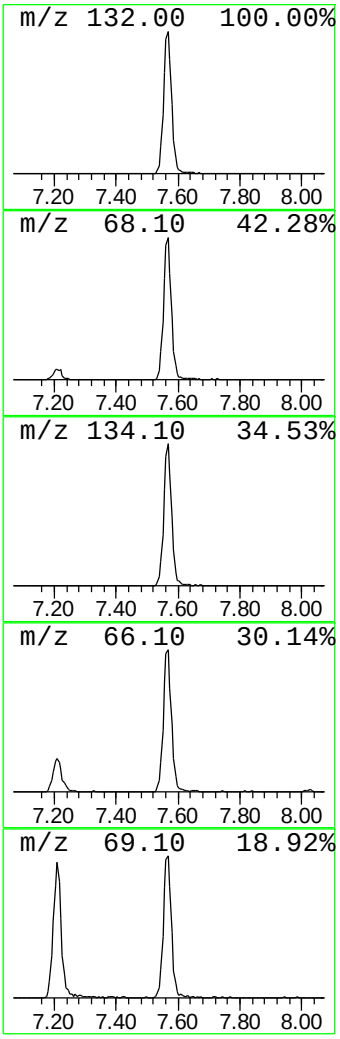
****

Peak Number 3 unknown7.57 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.57	99.49 ng	1330280	1,4-Dichlorobenzene-d4	8.03

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3-Cyclopentanedione, 2-chloro-	132	C5H5ClO2	014203-19-1	35
2	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	27
3	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
4	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
5	Imidazole, 4,5-dicyano-1-methyl-	132	C6H4N4	019485-35-9	25





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Operator : JU
Sample : K5615-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : RBR-29

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG102119.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

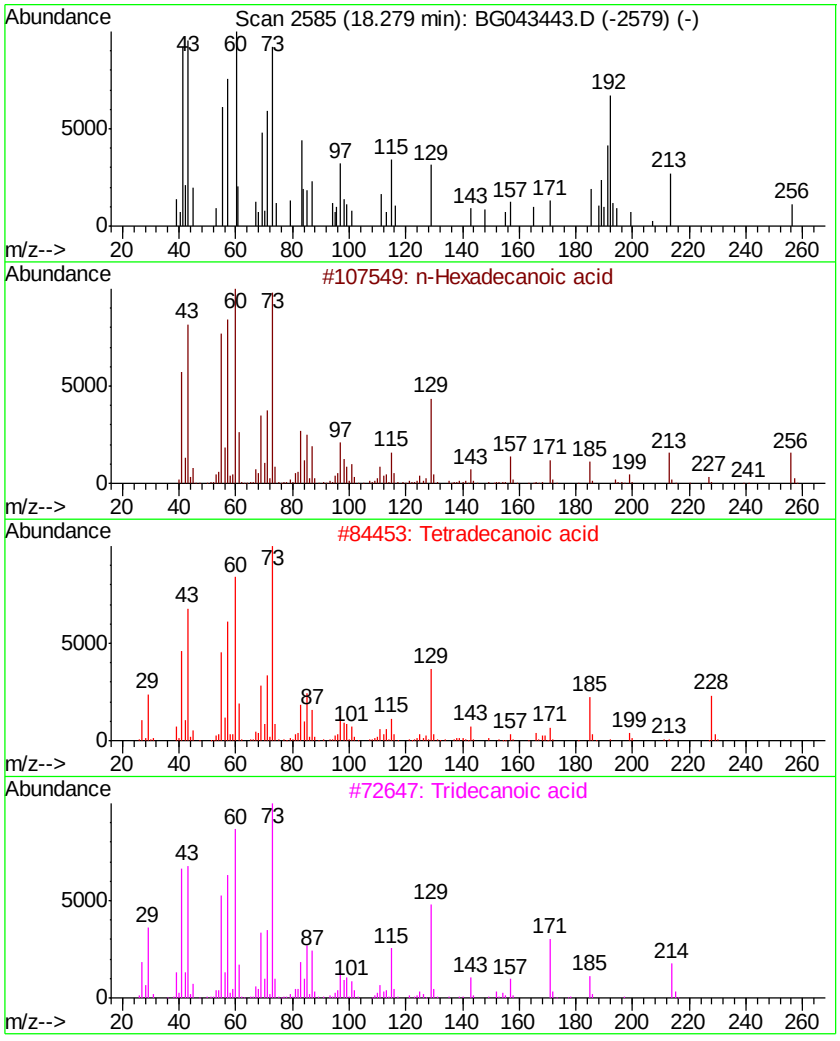
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

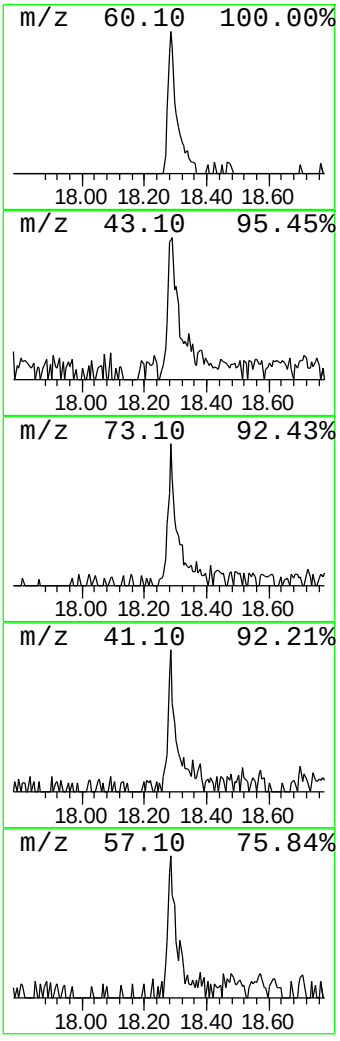
****

Peak Number 5 n-Hexadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.28	2.45 ng	72562	Phenanthrene-d10	17.40

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	97
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	92
3	Tridecanoic acid	214	C13H26O2	000638-53-9	86
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	70
5	Dodecanoic acid	200	C12H24O2	000143-07-7	52





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Sample : K5615-01
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ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : RBR-29

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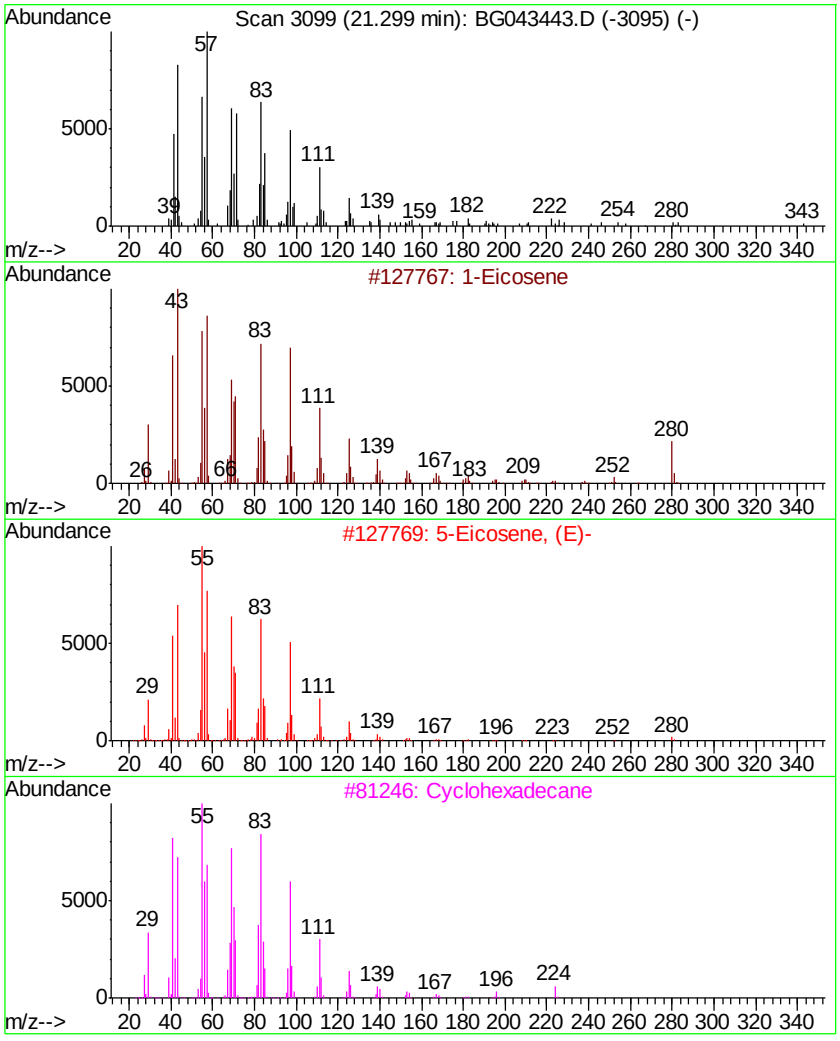
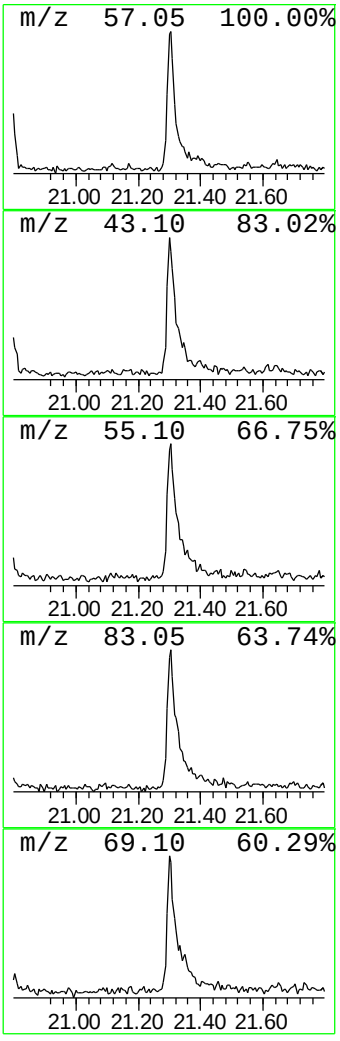
****

Peak Number 6 1-Eicosene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.30	6.04 ng	251779	Chrysene-d12	21.66

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Eicosene	280	C20H40	003452-07-1	93
2	5-Eicosene, (E)-	280	C20H40	074685-30-6	92
3	Cyclohexadecane	224	C16H32	000295-65-8	92
4	Tricosyl heptafluorobutyrate	536	C27H47F7O2	1000351-83-4	91
5	1-Hexadecanesulfonyl chloride	324	C16H33ClO2S	038775-38-1	90





Library Search Compound Report

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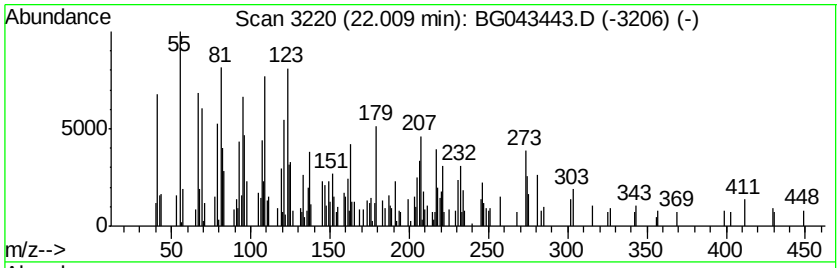
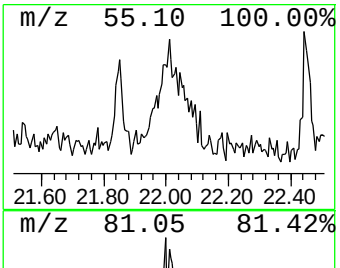
****

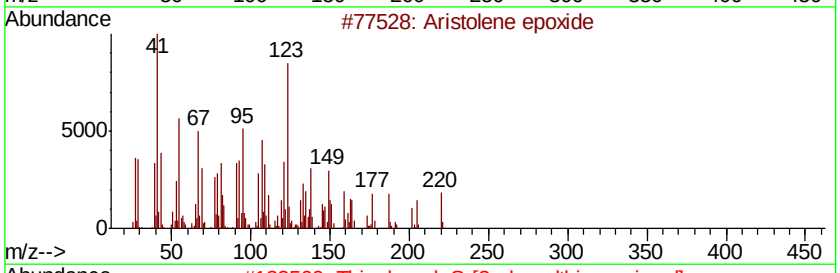
Peak Number 7 unknown22.01 Concentration Rank 6

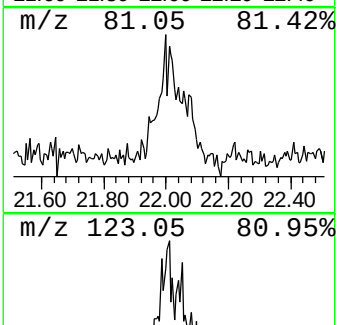
R.T.	EstConc	Area	Relative to ISTD	R.T.
22.01	5.28 ng	220256	Chrysene-d12	21.66

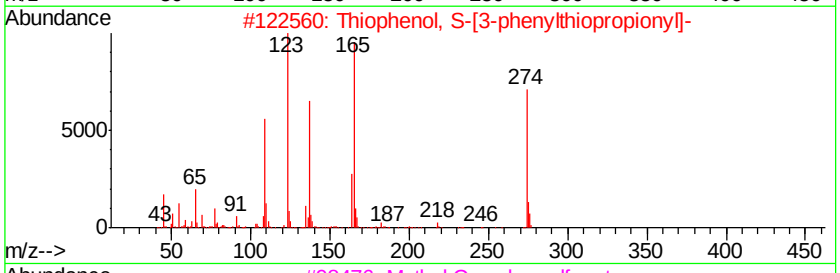
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Aristolene epoxide	220	C15H24O	1000151-48-9	44
2	Thiophenol, S-[3-phenylthiopropi...	274	C15H14OS2	087797-69-1	43
3	Methyl Camphorsulfonates	246	C11H18O4S	046471-67-4	38
4	Davana ether	234	C15H22O2	035470-57-6	35
5	3-Cyclohexene-1-carboxaldehyde, ...	152	C10H16O	040702-26-9	25

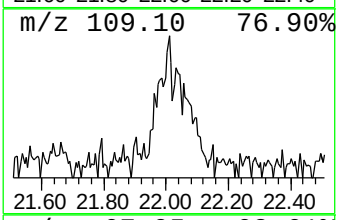


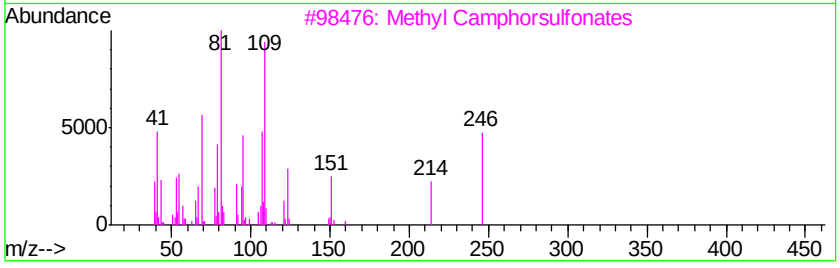


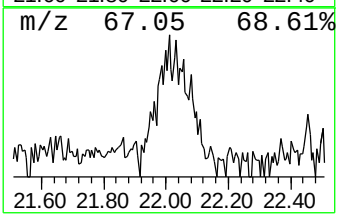












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TIC Library : C:\Database\NIST11.L
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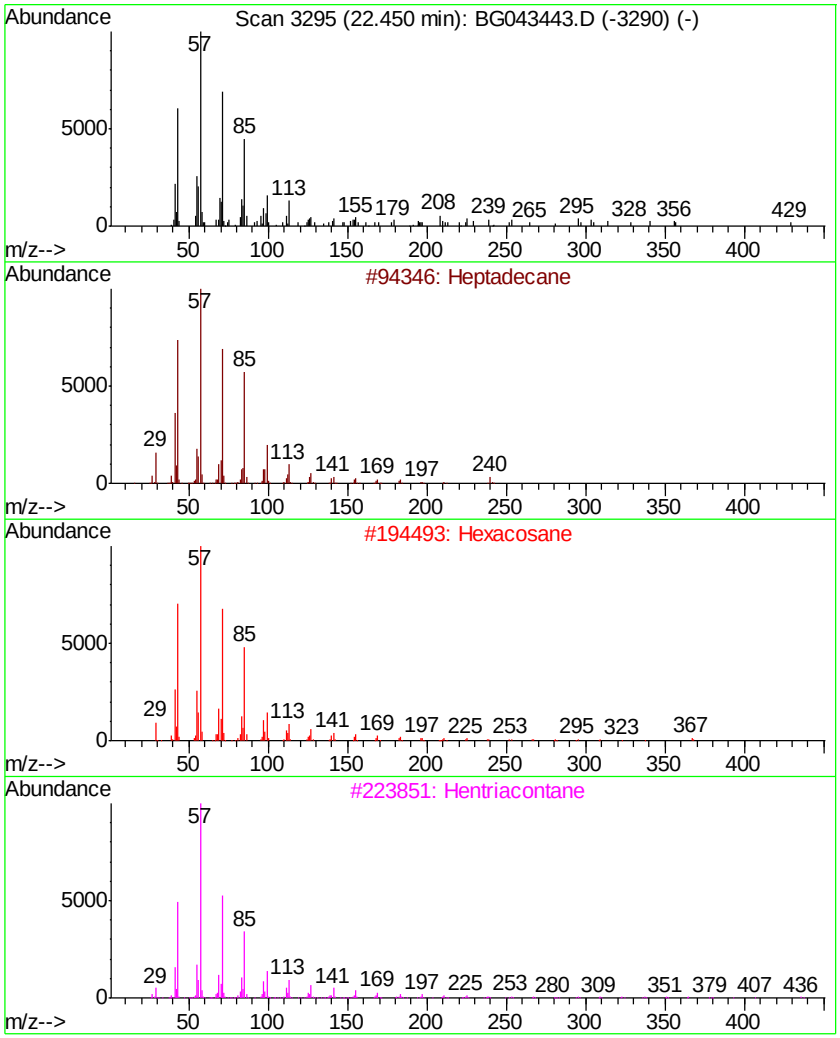
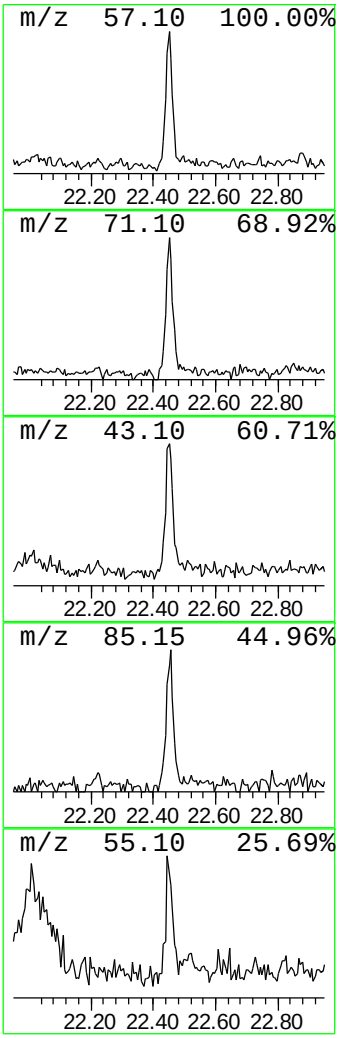
****

Peak Number 8 Heptadecane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.45	2.03 ng	84480	Chrysene-d12	21.66

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane	240	C17H36	000629-78-7	87
2	Hexacosane	366	C26H54	000630-01-3	87
3	Hentriacontane	437	C31H64	000630-04-6	86
4	Pentacosane	352	C25H52	000629-99-2	86
5	Eicosane, 2-methyl-	296	C21H44	001560-84-5	80





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

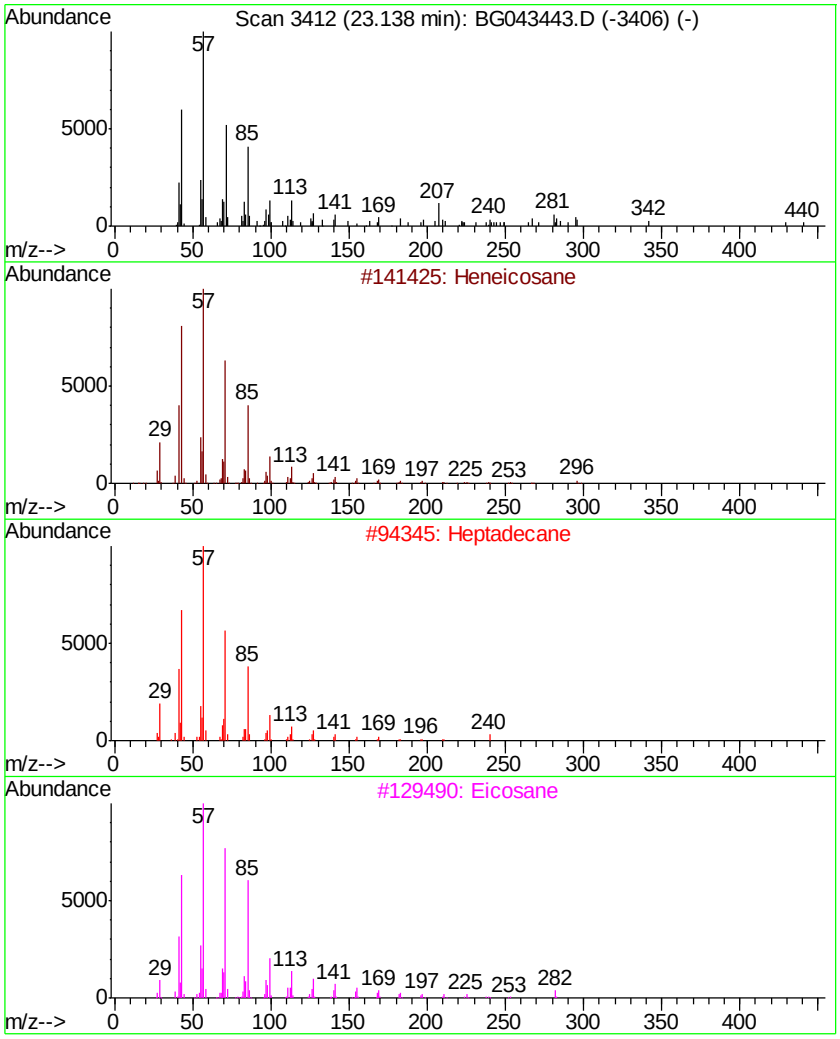
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

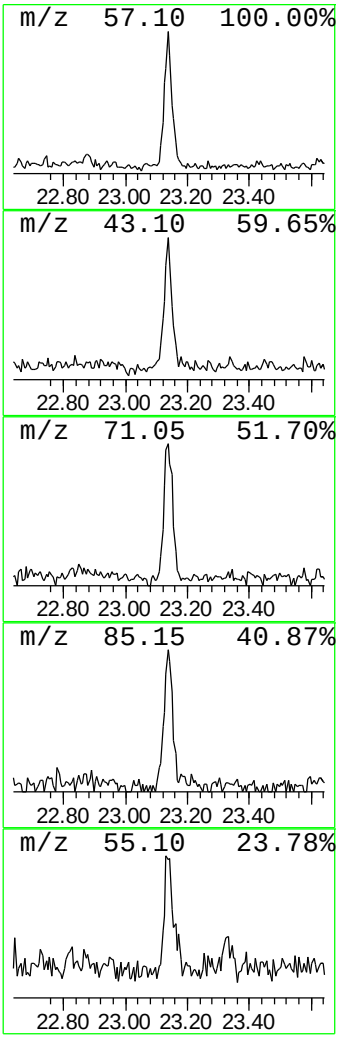
****

Peak Number 9 Heneicosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.14	2.35 ng	97949	Chrysene-d12	21.66

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	98
2	Heptadecane	240	C17H36	000629-78-7	96
3	Eicosane	282	C20H42	000112-95-8	93
4	Hentriacontane	437	C31H64	000630-04-6	86
5	Heptacosane	380	C27H56	000593-49-7	70





Tentatively Identified Compound (LSC) summary

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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
Butane, 2-methoxy...	3.20	11.3	ng	150744	1	8.03	267426	20.0
2-Pentanone, 4-hy...	5.13	16.4	ng	219850	1	8.03	267426	20.0
unknown7.57	7.57	99.5	ng	1330280	1	8.03	267426	20.0
n-Hexadecanoic acid	18.28	2.5	ng	72562	4	17.40	593431	20.0
1-Eicosene	21.30	6.0	ng	251779	5	21.66	834193	20.0
unknown22.01	22.01	5.3	ng	220256	5	21.66	834193	20.0
Heptadecane	22.45	2.0	ng	84480	5	21.66	834193	20.0
Heneicosane	23.14	2.4	ng	97949	5	21.66	834193	20.0