LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG082922\
Data File : BG054771.D
Acq On : 29 Aug 2022 13:52
Operator : CG/JU
Sample : N4355-09
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW-35

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-BG082522.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG054771.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.208	319	327	338	rBV	73525	118593	3.07%	0.860%
2	5.684	402	408	419	rVB	193719	314273	8.12%	2.280%
3	7.288	674	681	692	rVB	130969	230704	5.96%	1.674%
4	8.146	821	827	835	rBV	157900	272129	7.04%	1.974%
5	8.522	884	891	898	rVB2	25755	46702	1.21%	0.339%
6	9.321	1019	1027	1035	rBV	514468	935110	24.17%	6.785%
7	10.972	1297	1308	1315	rBV	224010	405403	10.48%	2.941%
8	13.405	1713	1722	1730	rBV	1524935	2370217	61.28%	17.197%
9	14.780	1949	1956	1965	rVB	381590	589142	15.23%	4.274%
10	16.260	2202	2208	2223	rBV	693185	1124557	29.07%	8.159%
11	17.523	2416	2423	2432	rBV	484151	755294	19.53%	5.480%
12	18.170	2528	2533	2539	rBV	89499	113511	2.93%	0.824%
13	19.333	2725	2731	2735	rVB3	37860	51083	1.32%	0.371%
14	19.468	2749	2754	2758	rBV	32768	40204	1.04%	0.292%
15	20.126	2859	2866	2879	rBV	2946800	3868099	100.00%	28.065%
16	20.414	2911	2915	2919	rVB	39896	45806	1.18%	0.332%
17	20.914	2995	3000	3003	rBV2	63371	83084	2.15%	0.603%
18	21.431	3083	3088	3098	rBV	132235	218668	5.65%	1.587%
19	21.683	3127	3131	3139	rVB	76791	106393	2.75%	0.772%
20	21.812	3146	3153	3164	rVB2	469106	811535	20.98%	5.888%
21	21.995	3180	3184	3191	rVB	57437	82983	2.15%	0.602%
22	22.629	3287	3292	3299	rVB2	49844	84955	2.20%	0.616%
23	23.352	3409	3415	3426	rVB	40303	82703	2.14%	0.600%
24	23.558	3444	3450	3458	rVB	39122	83815	2.17%	0.608%
25	24.204	3553	3560	3567	rVB2	28068	60866	1.57%	0.442%
26	25.179	3714	3726	3739	rBV2	282660	886893	22.93%	6.435%

Sum of corrected areas: 13782722

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG082922\
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Operator : CG/JU
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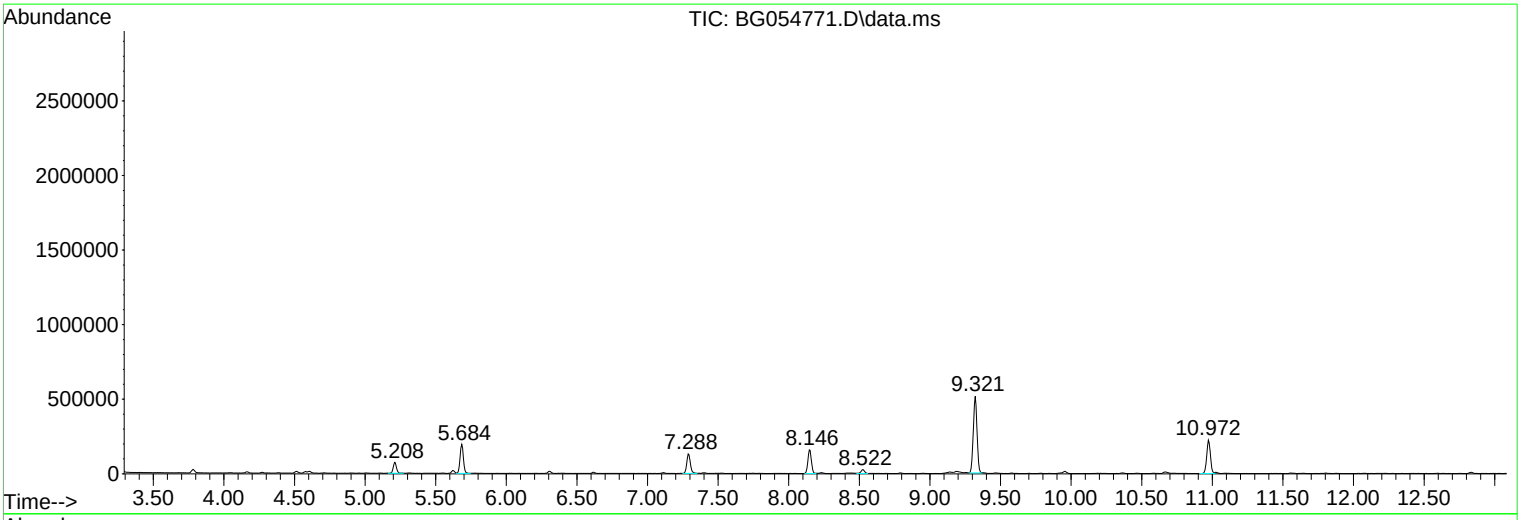
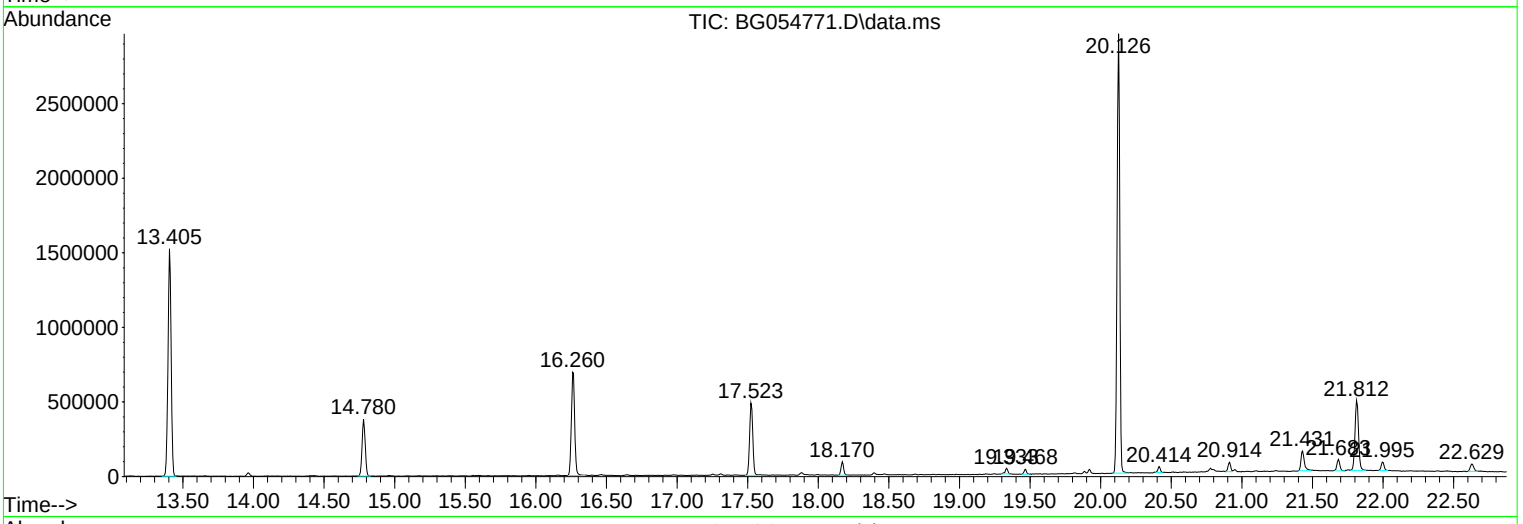
Misc :
ALS Vial : 7 Sample Multiplier: 1

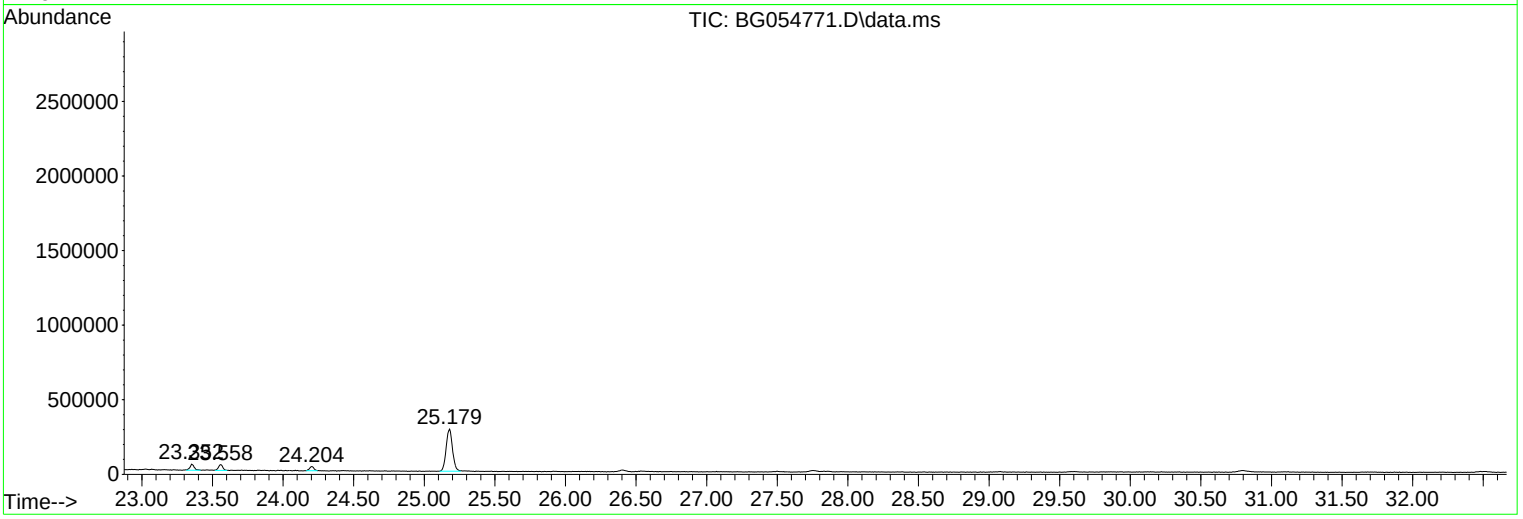
Instrument :
BNA_G
ClientSampleId :
MW-35

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG082522.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 : BG054771.D
Acq On : 29 Aug 2022 13:52
Operator : CG/JU
Sample : N4355-09
Misc :
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Instrument :
BNA_G
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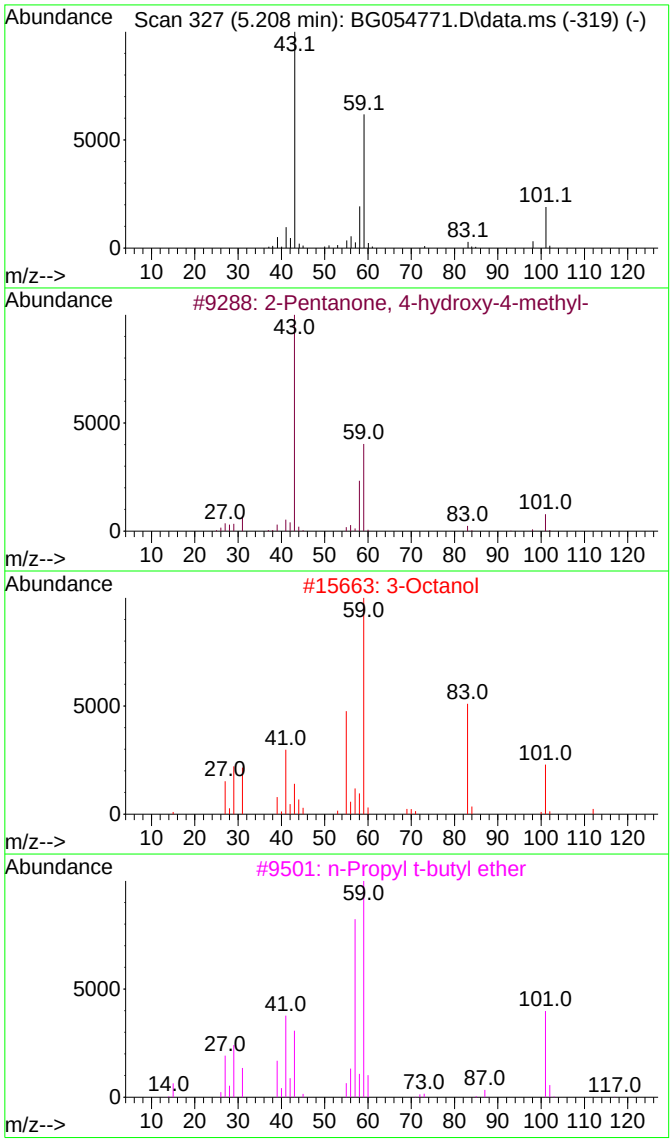
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG082522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

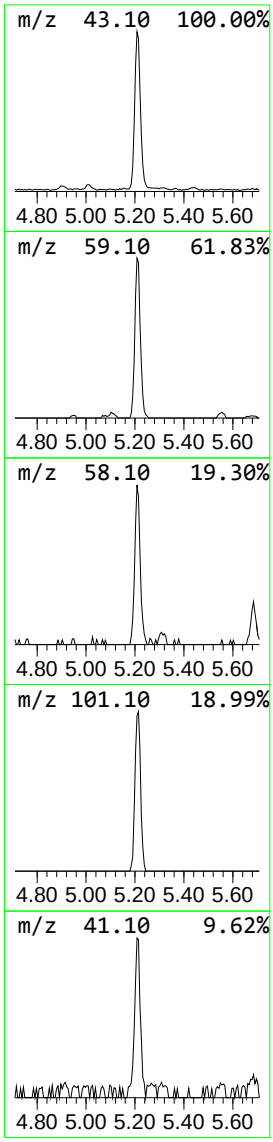
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.208	8.72 ng	118593	1,4-Dichlorobenzene-d4	8.152

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	45
2	3-Octanol	130	C8H18O	000589-98-0	28
3	n-Propyl t-butyl ether	116	C7H16O	1000334-81-9	28
4	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	25
5	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23





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Data File : BG054771.D
Acq On : 29 Aug 2022 13:52
Operator : CG/JU
Sample : N4355-09
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW-35

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG082522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

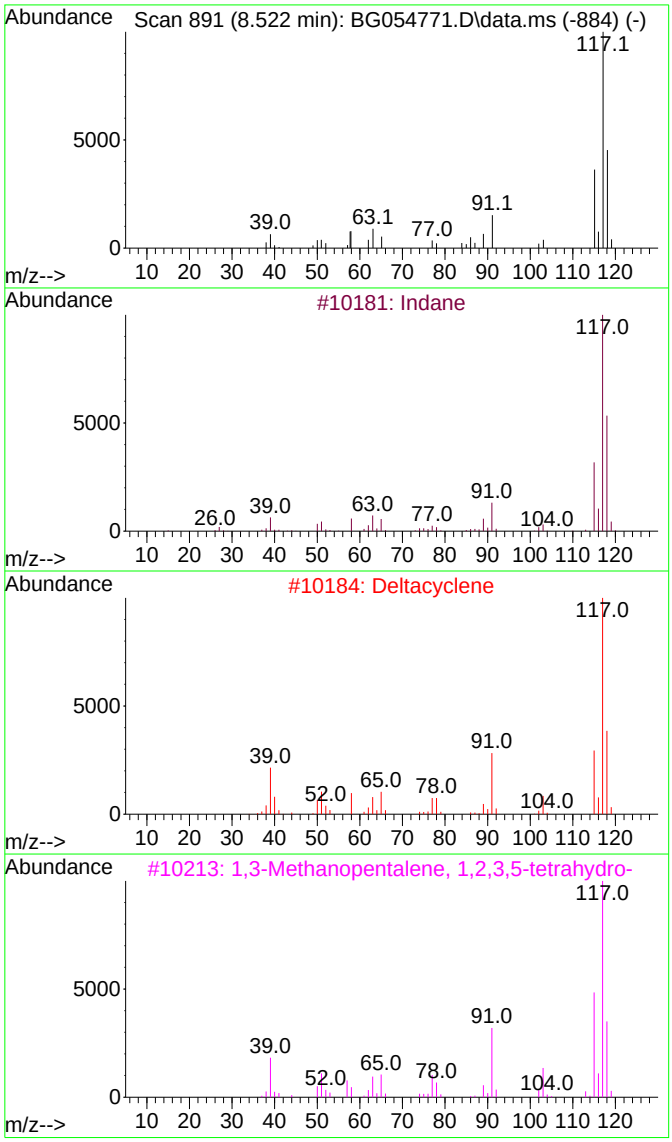
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

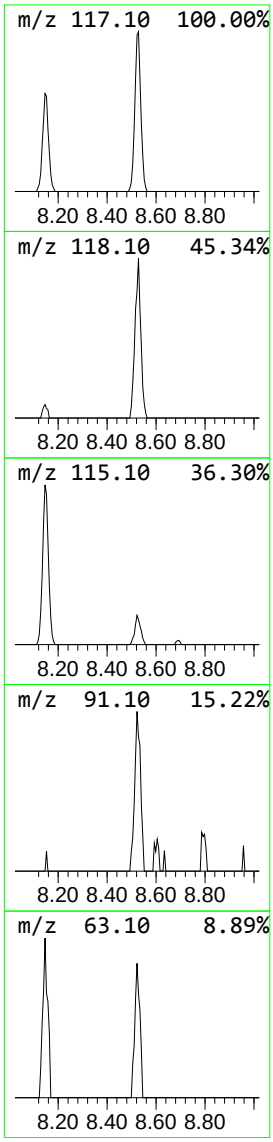
****

Peak Number 2 Indane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.522	3.43 ng	46702	1,4-Dichlorobenzene-d4	8.152

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Indane	118	C9H10	000496-11-7	83
2	Deltacyclene	118	C9H10	007785-10-6	64
3	1,3-Methanopentalene, 1,2,3,5-te...	118	C9H10	128600-88-4	59
4	Tetracyclo[3.3.1.0(2,8).0(4,6)]-...	118	C9H10	1000191-13-7	59
5	Benzeneethanol, .beta.-ethenyl-	148	C10H12O	006052-63-7	53





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Acq On : 29 Aug 2022 13:52
Operator : CG/JU
Sample : N4355-09
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW-35

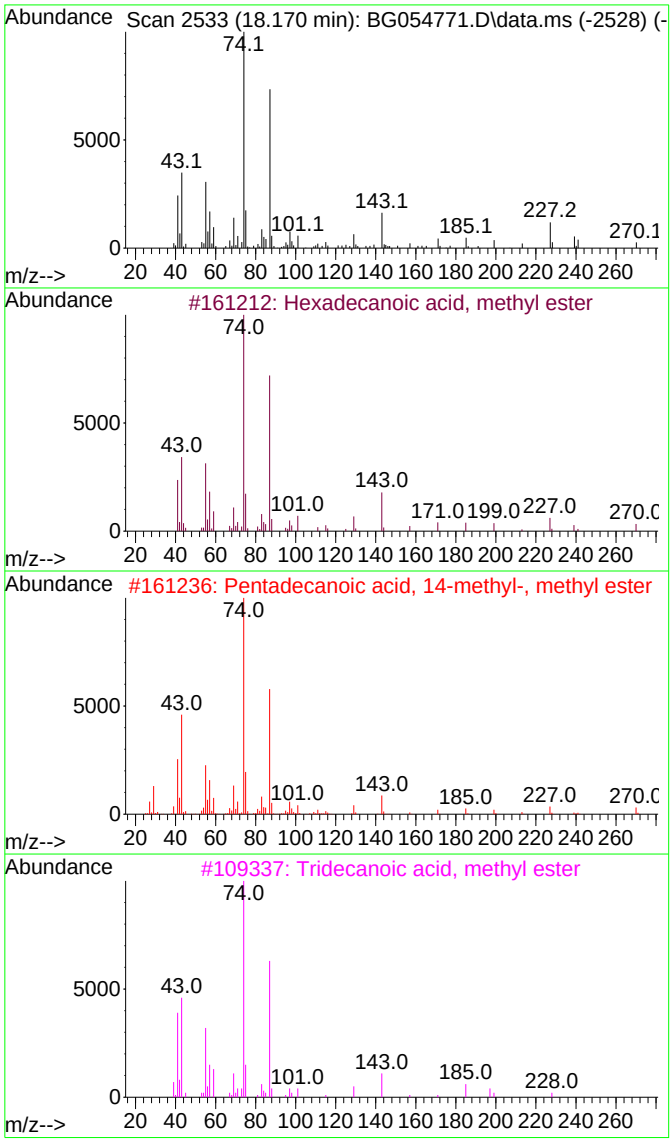
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG082522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

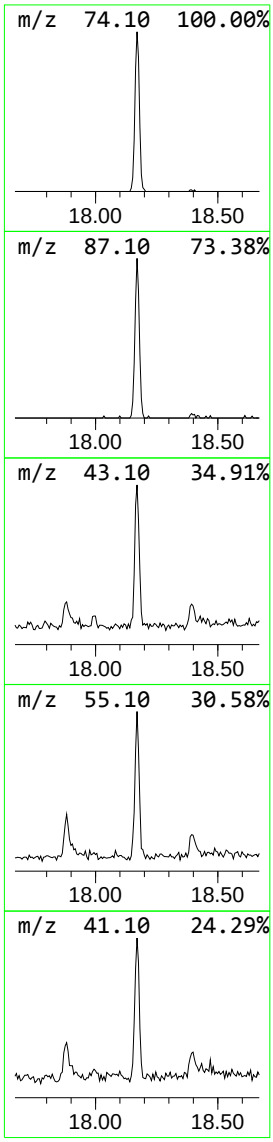
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Hexadecanoic acid, methyl e... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.170	3.01 ng	113511	Phenanthrene-d10	17.523

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	98
2	Pentadecanoic acid, 14-methyl-, ...	270	C17H34O2	005129-60-2	96
3	Tridecanoic acid, methyl ester	228	C14H28O2	001731-88-0	90
4	Pentadecanoic acid, methyl ester	256	C16H32O2	007132-64-1	86
5	Methyl tetradecanoate	242	C15H30O2	000124-10-7	83





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Data File : BG054771.D
Acq On : 29 Aug 2022 13:52
Operator : CG/JU
Sample : N4355-09
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW-35

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG082522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

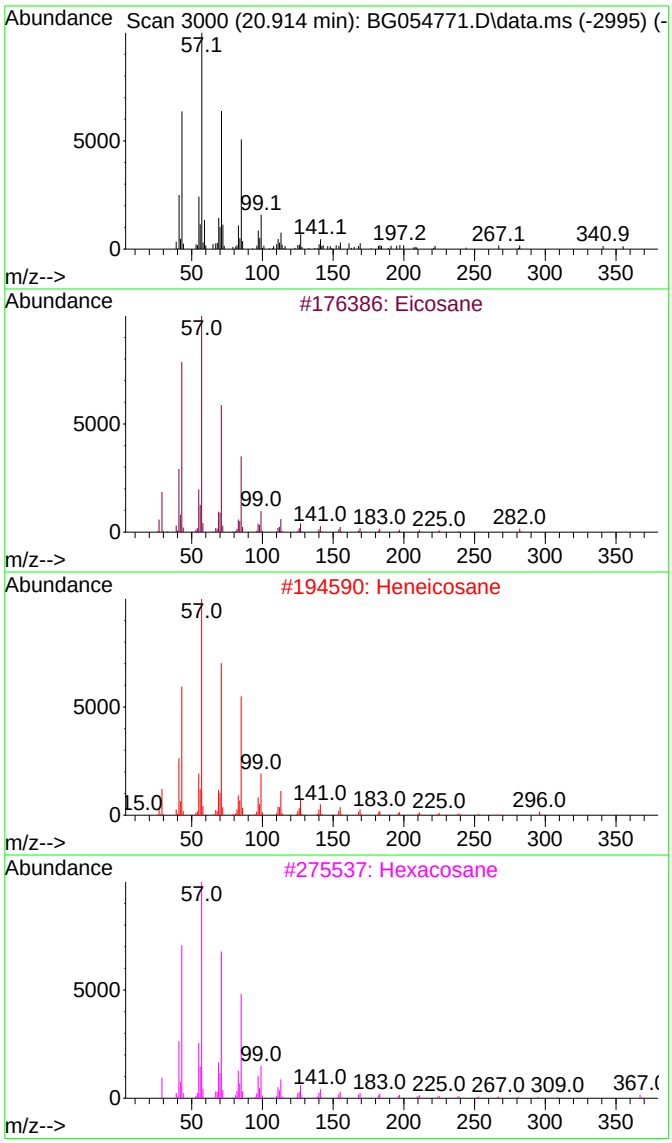
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

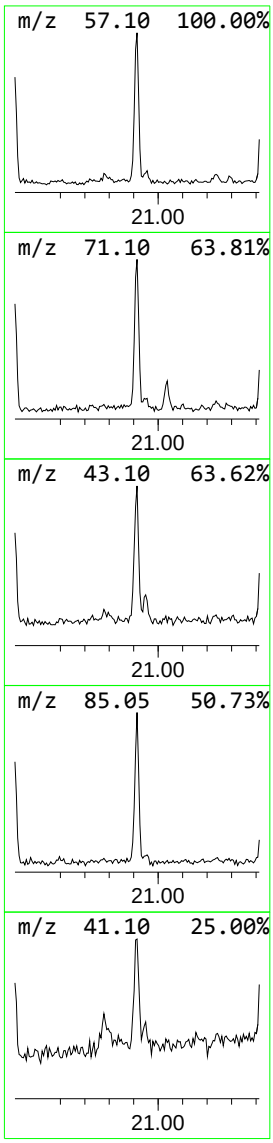
****

Peak Number 4 Eicosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.914	2.05 ng	83084	Chrysene-d12	21.813

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	97
2	Heneicosane	296	C21H44	000629-94-7	81
3	Hexacosane	366	C26H54	000630-01-3	81
4	Dodecane, 2-methyl-	184	C13H28	001560-97-0	76
5	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	74





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG082922\
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Operator : CG/JU
Sample : N4355-09
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW-35

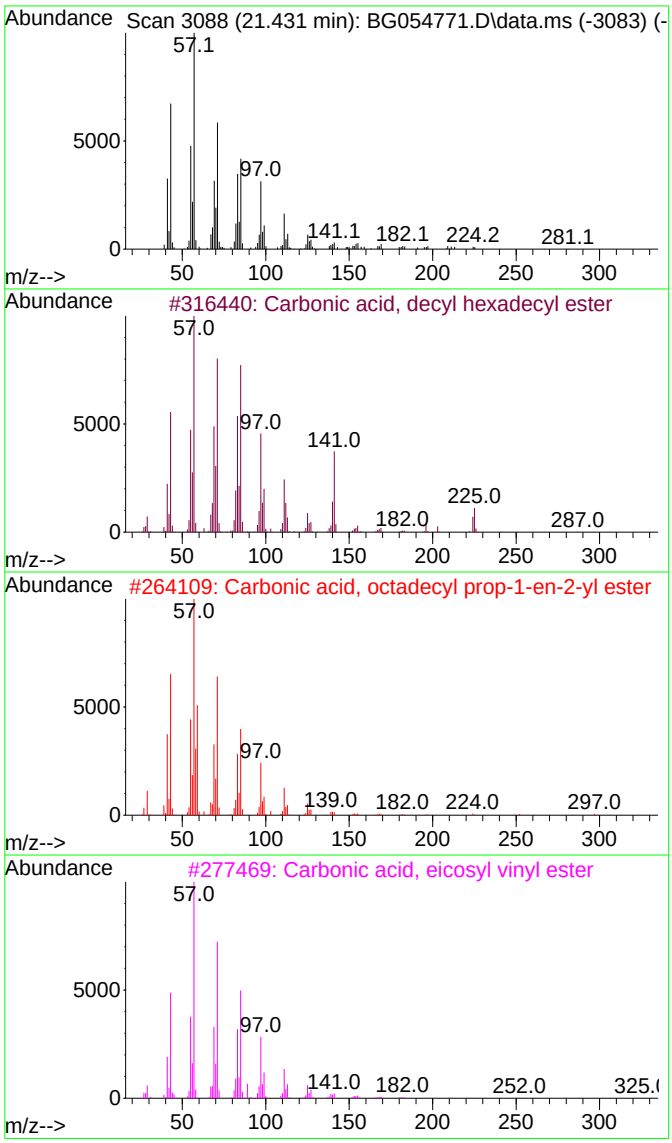
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG082522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

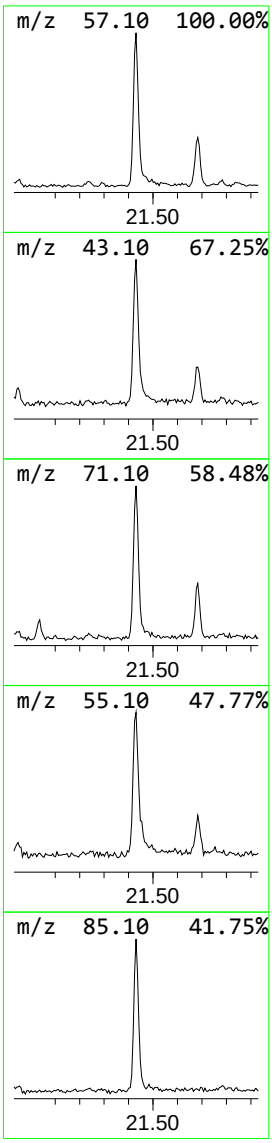
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Carbonic acid, decyl hexade... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.431	5.39 ng	218668	Chrysene-d12	21.813

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Carbonic acid, decyl hexadecyl e...	426	C27H54O3	1000383-16-5	91
2	Carbonic acid, octadecyl prop-1-...	354	C22H42O3	1000383-11-5	91
3	Carbonic acid, eicosyl vinyl ester	368	C23H44O3	1000382-54-3	91
4	Carbonic acid, hexadecyl prop-1-...	326	C20H38O3	1000382-90-3	91
5	Carbonic acid, decyl tridecyl ester	384	C24H48O3	1000383-16-2	91





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Data File : BG054771.D
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Sample : N4355-09
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BNA_G
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG082522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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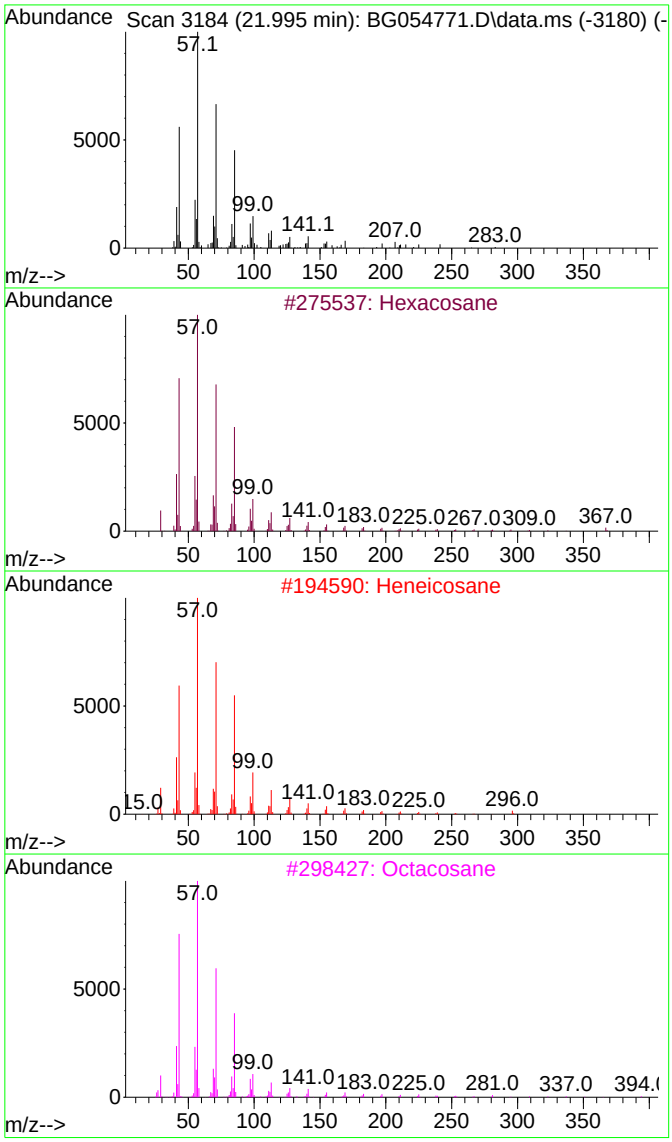
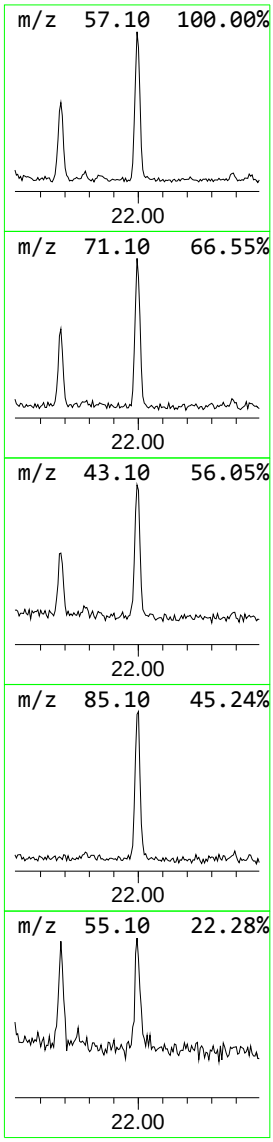
****

Peak Number 6 Hexacosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.995	2.05 ng	82983	Chrysene-d12	21.813

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosane	366	C26H54	000630-01-3	91
2	Heneicosane	296	C21H44	000629-94-7	91
3	Octacosane	394	C28H58	000630-02-4	91
4	Tetracosane	338	C24H50	000646-31-1	91
5	Octacosane, 2-methyl-	408	C29H60	001560-98-1	91





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Sample : N4355-09
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW-35

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG082522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

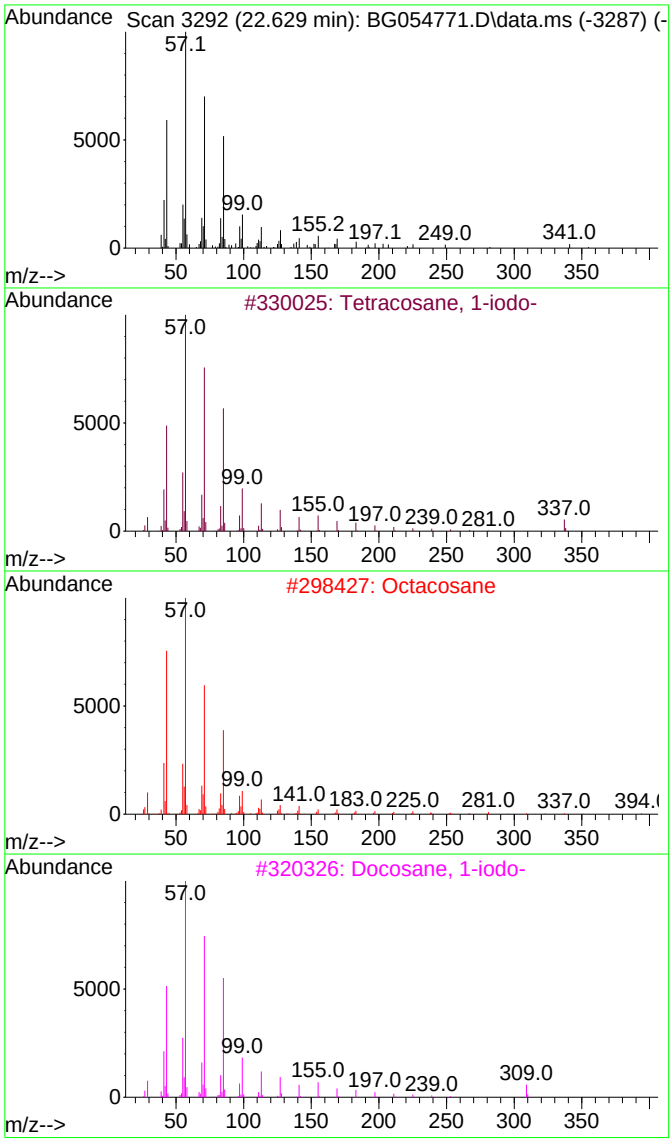
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

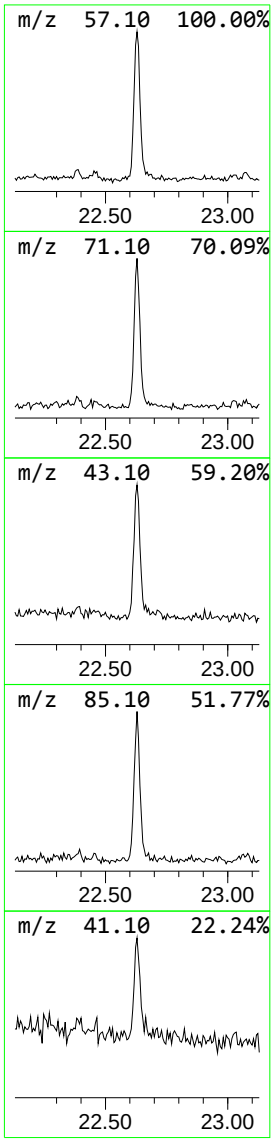
****

Peak Number 7 Tetracosane, 1-iodo- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.629	2.09 ng	84955	Chrysene-d12	21.813

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetracosane, 1-iodo-	464	C24H49I	1000406-32-0	91
2	Octacosane	394	C28H58	000630-02-4	91
3	Docosane, 1-iodo-	436	C22H45I	1000406-31-9	91
4	Triacontane	422	C30H62	000638-68-6	91
5	Docosane	310	C22H46	000629-97-0	91





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BNA_G
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

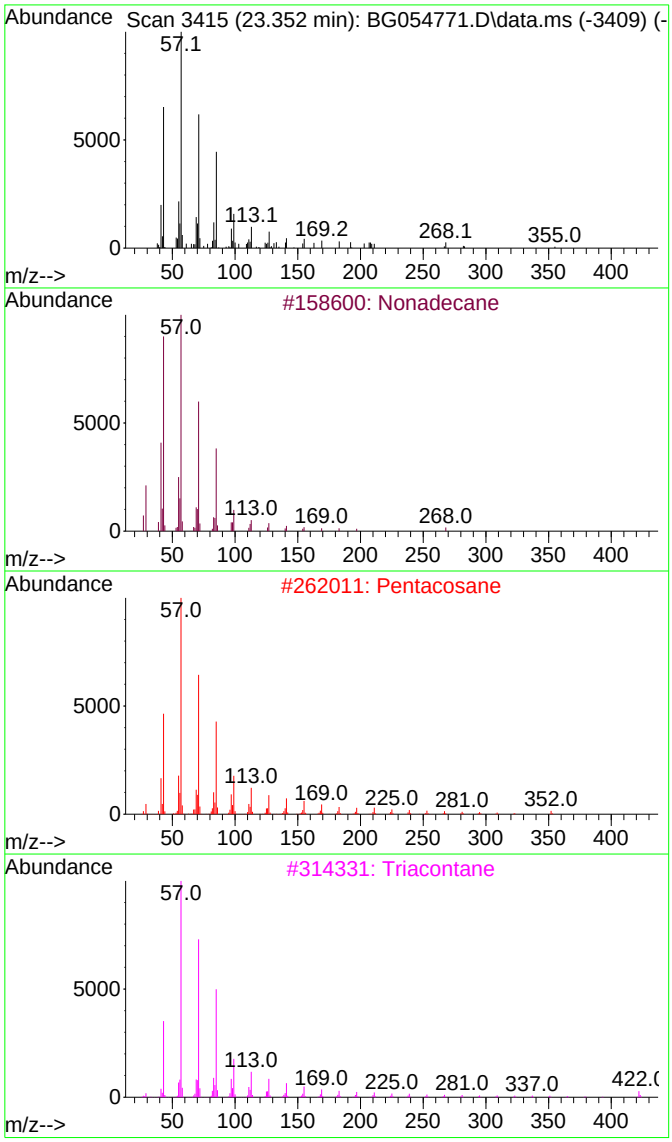
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

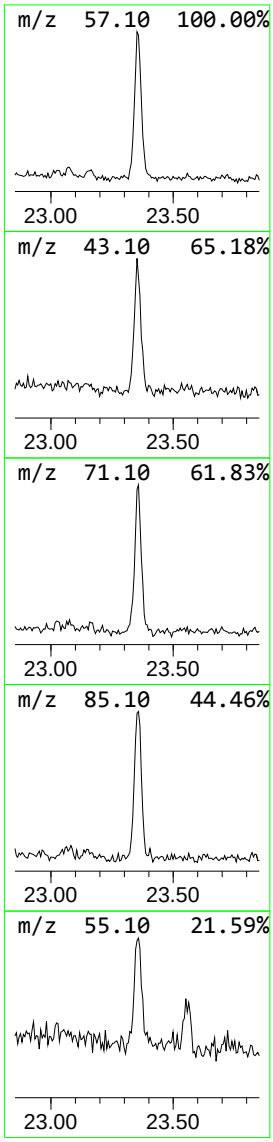
****

Peak Number 8 Nonadecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.352	2.04 ng	82703	Chrysene-d12	21.813

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonadecane	268	C19H40	000629-92-5	94
2	Pentacosane	352	C25H52	000629-99-2	91
3	Triacontane	422	C30H62	000638-68-6	91
4	4-Methylheneicosane	310	C22H46	025117-29-7	91
5	Tetracosane	338	C24H50	000646-31-1	91





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG082922\
Data File : BG054771.D
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Operator : CG/JU
Sample : N4355-09
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW-35

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG082522.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-...	5.208	8.7	ng	118593	1	8.152	272129	20.0
Indane	8.522	3.4	ng	46702	1	8.152	272129	20.0
Hexadecanoic ac...	18.170	3.0	ng	113511	4	17.523	755294	20.0
Eicosane	20.914	2.0	ng	83084	5	21.813	811535	20.0
Carbonic acid, ...	21.431	5.4	ng	218668	5	21.813	811535	20.0
Hexacosane	21.995	2.0	ng	82983	5	21.813	811535	20.0
Tetracosane, 1-...	22.629	2.1	ng	84955	5	21.813	811535	20.0
Nonadecane	23.352	2.0	ng	82703	5	21.813	811535	20.0