LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG052720\
Data File : BG045490.D
Acq On : 28 May 2020 00:23
Operator : CG/JU
Sample : L2745-16
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : NM36-COMP-2020-0-6

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-BG051520.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	3.117	3	5	18	rVB	163786	221305	5.25%	0.690%
2	5.560	413	421	435	rBV	886311	1535204	36.41%	4.790%
3	7.176	688	696	708	rBV	1037447	1900026	45.06%	5.928%
4	7.957	821	829	840	rBV	366544	653250	15.49%	2.038%
5	8.286	876	885	898	rBV	940628	1685528	39.97%	5.259%
6	9.120	1019	1027	1041	rBV	713100	1352610	32.08%	4.220%
7	10.765	1297	1307	1314	rBV	514910	926399	21.97%	2.890%
8	13.227	1718	1726	1736	rBV	2053894	3402267	80.69%	10.615%
9	14.049	1859	1866	1872	rBV	240453	370162	8.78%	1.155%
10	14.601	1952	1960	1967	rBV	847755	1376483	32.64%	4.295%
11	16.099	2205	2215	2224	rBV	1658979	2575433	61.08%	8.035%
12	17.350	2421	2428	2432	rBV	931672	1446391	34.30%	4.513%
13	17.391	2432	2435	2442	rVB	168591	256562	6.08%	0.800%
14	17.480	2447	2450	2455	rVB2	36190	56814	1.35%	0.177%
15	18.226	2570	2577	2579	rBV	34614	57618	1.37%	0.180%
16	18.255	2579	2582	2585	rBV3	44211	59002	1.40%	0.184%
17	18.419	2605	2610	2614	rBV3	55365	107079	2.54%	0.334%
18	19.277	2751	2756	2761	rBV4	31376	64801	1.54%	0.202%
19	19.348	2763	2768	2772	rVV	166500	234752	5.57%	0.732%
20	19.401	2772	2777	2783	rVB	468084	683604	16.21%	2.133%
21	19.765	2829	2839	2847	rBV	406098	768793	18.23%	2.399%
22	19.841	2848	2852	2856	rBV5	24263	43041	1.02%	0.134%
23	19.964	2867	2873	2879	rBV	3087045	4216656	100.00%	13.156%
24	20.082	2891	2893	2901	rVB4	28405	57027	1.35%	0.178%
25	20.258	2920	2923	2932	rVB3	81600	134736	3.20%	0.420%
26	20.358	2936	2940	2944	rVV2	43102	64772	1.54%	0.202%
27	20.605	2979	2982	2987	rBV4	34749	43745	1.04%	0.136%
28	21.269	3091	3095	3103	rVB5	221282	380877	9.03%	1.188%
29	21.609	3145	3153	3158	rBV3	894990	1815466	43.05%	5.664%
30	21.656	3158	3161	3173	rVB	205883	346233	8.21%	1.080%
31	21.809	3183	3187	3192	rVB2	140391	212940	5.05%	0.664%
32	22.408	3284	3289	3297	rVB4	238832	472038	11.19%	1.473%
33	23.090	3399	3405	3413	rVB	229549	439608	10.43%	1.372%
34	23.765	3514	3520	3529	rBV2	143788	457186	10.84%	1.426%

LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG052720\
Data File : BG045490.D
Acq On : 28 May 2020 00:23
Operator : CG/JU
Sample : L2745-16
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : NM36-COMP-2020-0-6

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-BG051520.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	23.877	3533	3539	3545	rVB2	282236	570644	13.53%	1.780%
36	24.611	3656	3664	3677	rVB2	128562	364264	8.64%	1.136%
37	24.764	3681	3690	3710	rVB3	478522	1909284	45.28%	5.957%
38	25.909	3877	3885	3894	rVB2	264915	789365	18.72%	2.463%

Sum of corrected areas: 32051965

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG052720\
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Acq On : 28 May 2020 00:23
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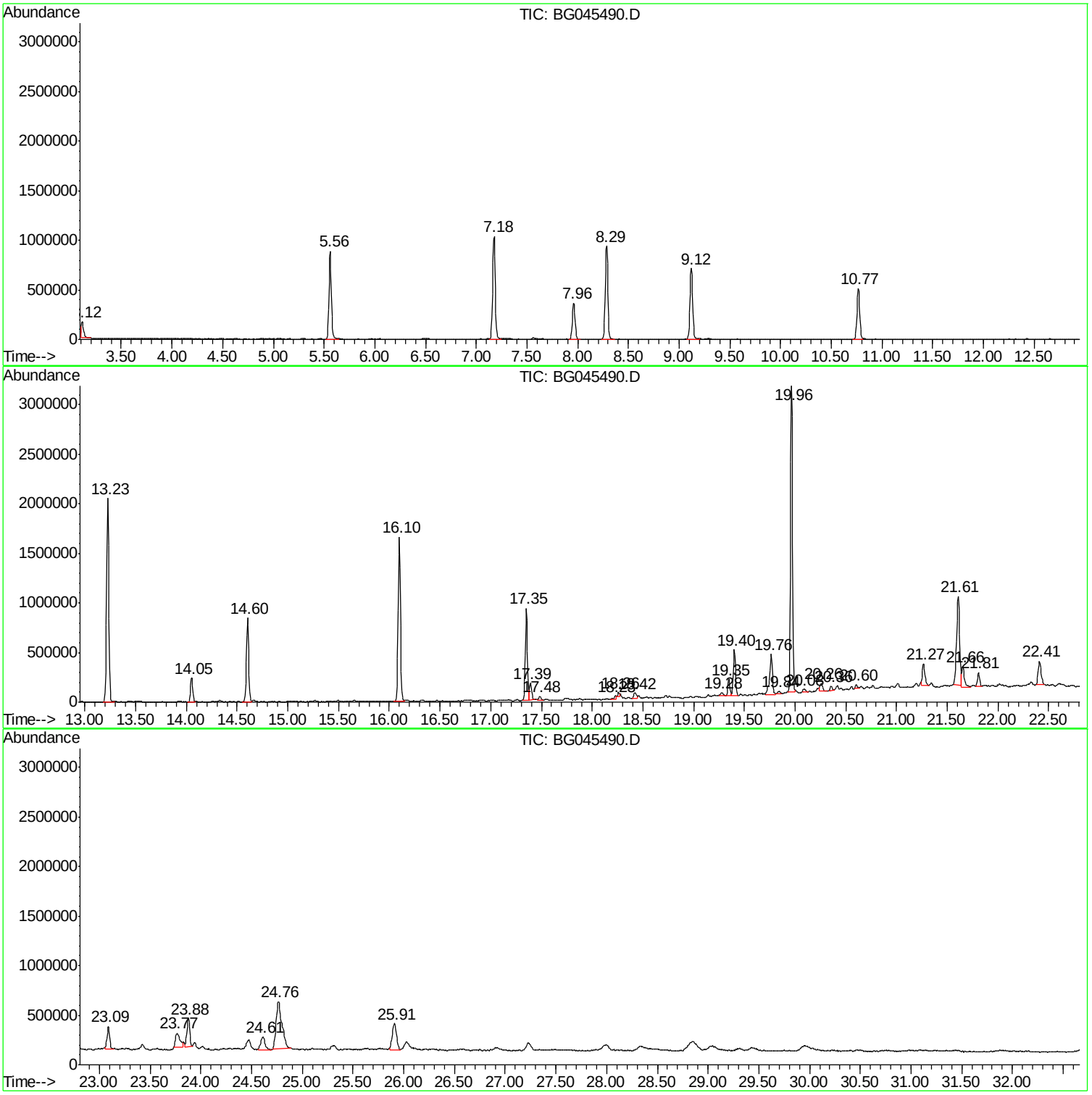
Sample : L2745-16
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
NM36-COMP-2020-0-6

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG051520.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG052720\
Data File : BG045490.D
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG051520.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

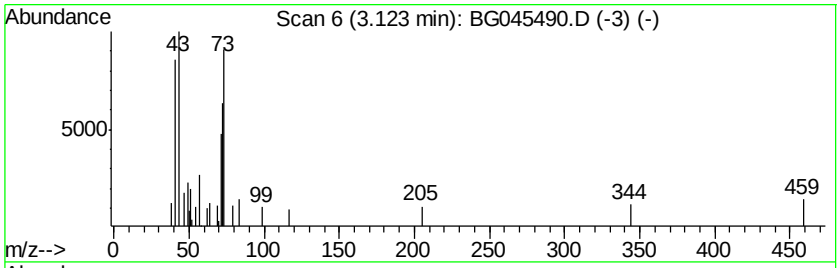
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

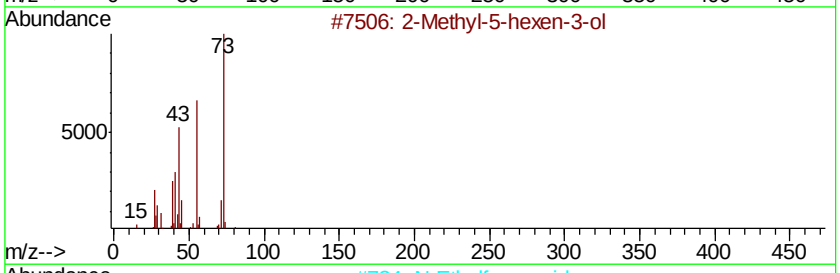
****

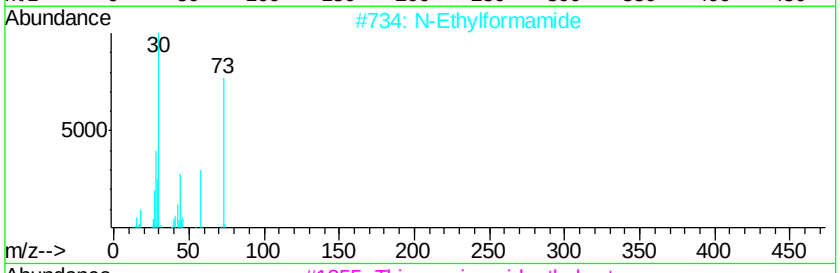
Peak Number 1 unknown3.12 Concentration Rank 3

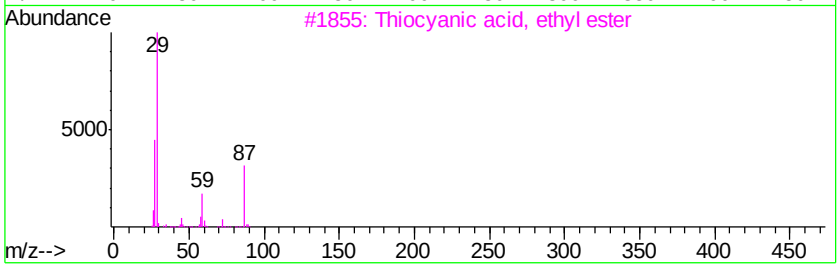
R.T.	EstConc	Area	Relative to ISTD	R.T.
3.12	6.78 ng	221305	1,4-Dichlorobenzene-d4	7.96

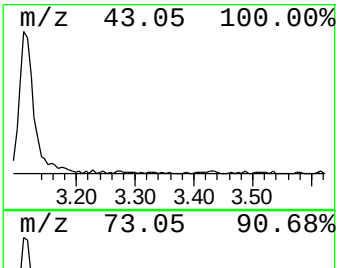
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	28
2	N-Ethylformamide	73	C3H7NO	000627-45-2	9
3	Thiocyanic acid, ethyl ester	87	C3H5NS	000542-90-5	9
4	3-Hexanol, 3-methyl-	116	C7H16O	000597-96-6	9
5	3-Hexanol, 2,4-dimethyl-	130	C8H18O	013432-25-2	9

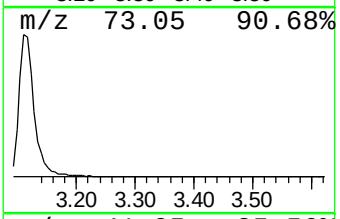


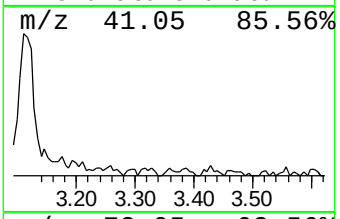


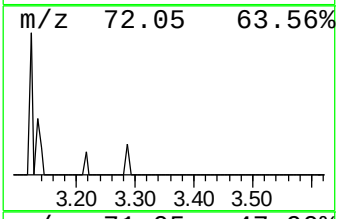


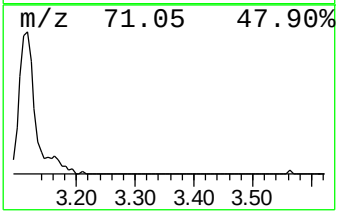












Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG052720\
Data File : BG045490.D
Acq On : 28 May 2020 00:23
Operator : CG/JU
Sample : L2745-16
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : NM36-COMP-2020-0-6

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG051520.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

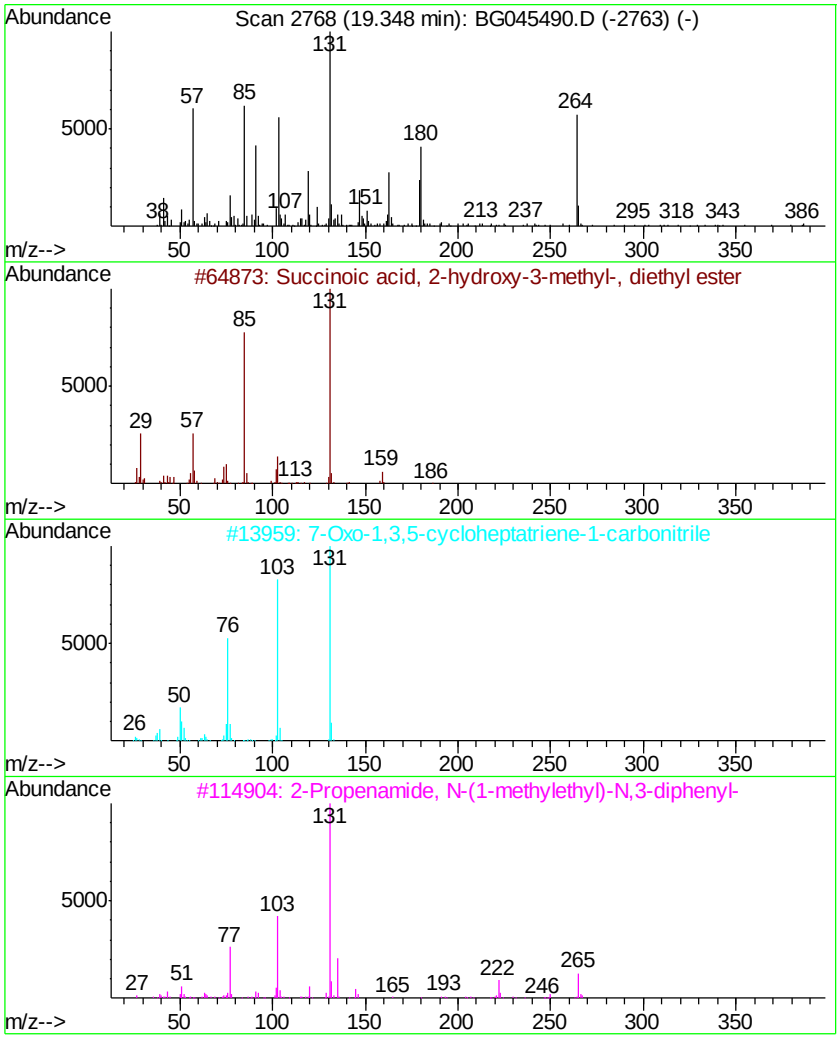
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

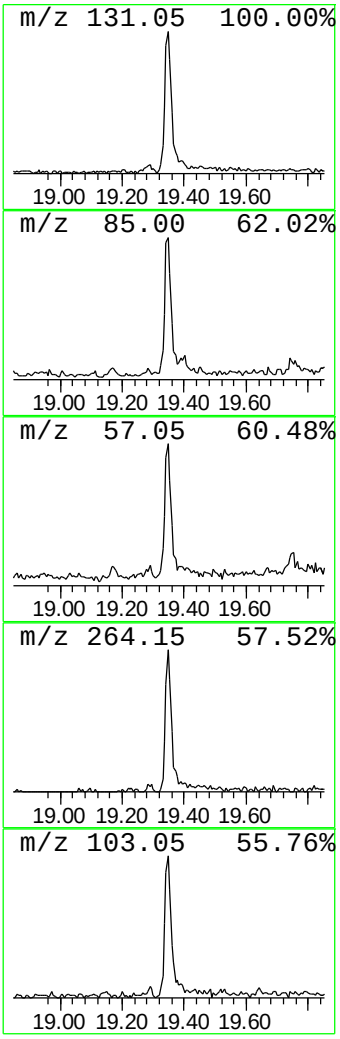
****

Peak Number 3 unknown19.35 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.35	3.25 ng	234752	Phenanthrene-d10	17.35

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Succinoic acid, 2-hydroxy-3-meth...	204	C9H16O5	1000196-85-6	27
2	7-Oxo-1,3,5-cycloheptatriene-1-c...	131	C8H5NO	000934-19-0	25
3	2-Propenamide, N-(1-methylethyl)...	265	C18H19NO	055044-37-6	22
4	Silane, ethoxytriethyl-	160	C8H20OSi	000597-67-1	22
5	p-Vinylbenzohydrazide	162	C9H10N2O	1000244-74-9	18





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG052720\
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ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : NM36-COMP-2020-0-6

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG051520.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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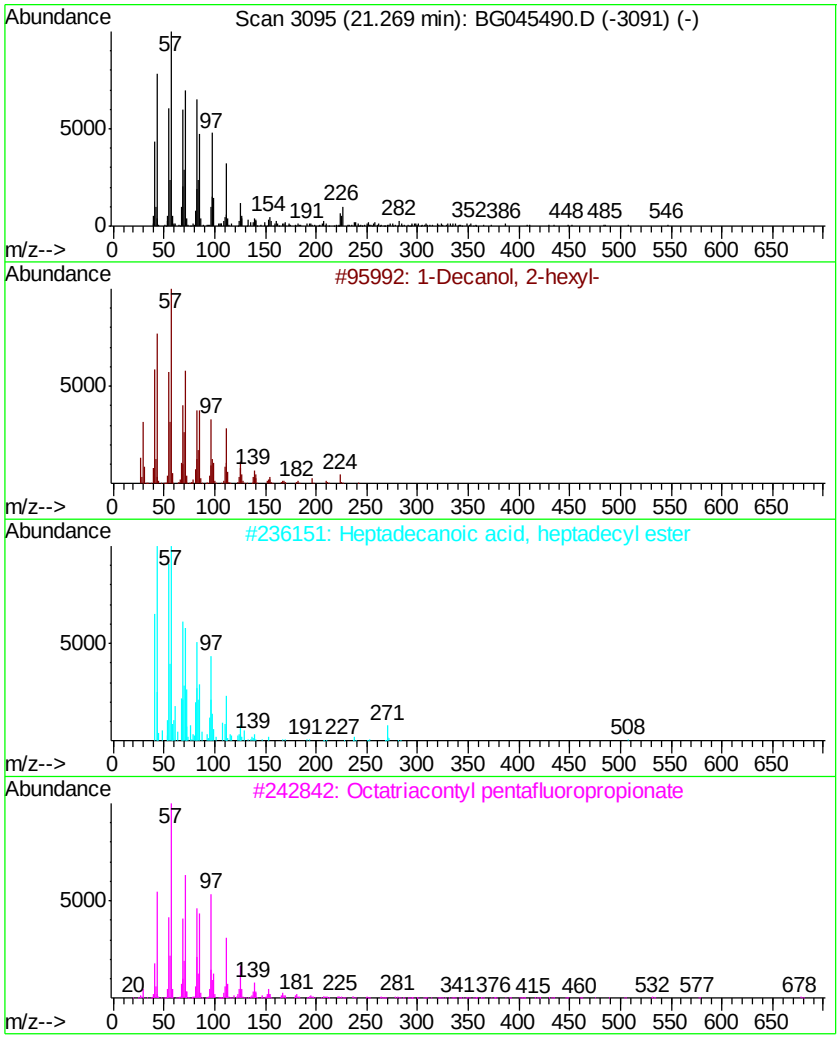
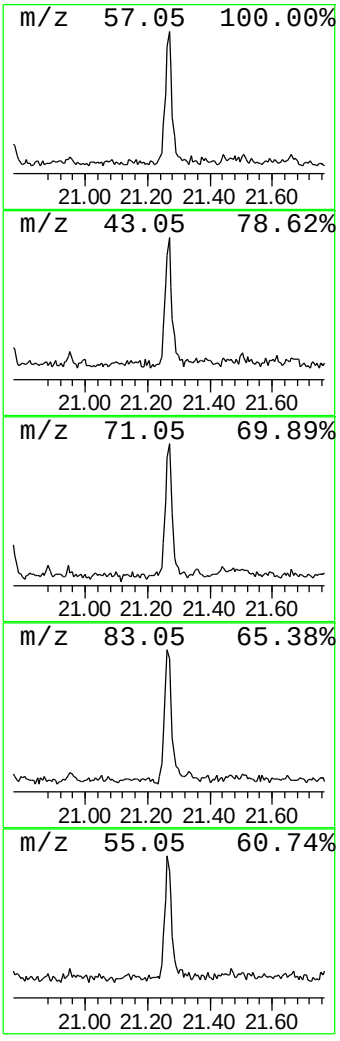
****

Peak Number 4 1-Decanol, 2-hexyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.27	4.20 ng	380877	Chrysene-d12	21.61

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Decanol, 2-hexyl-	242	C16H34O	002425-77-6	93
2	Heptadecanoic acid, heptadecyl e...	509	C34H68O2	036617-50-2	90
3	Octatriacontyl pentafluoropropio...	697	C41H77F5O2	1000351-89-1	80
4	3-Heptadecene, (Z)-	238	C17H34	1000141-67-3	64
5	1-Docosene	308	C22H44	001599-67-3	64





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG052720\
Data File : BG045490.D
Acq On : 28 May 2020 00:23
Operator : CG/JU
Sample : L2745-16
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : NM36-COMP-2020-0-6

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG051520.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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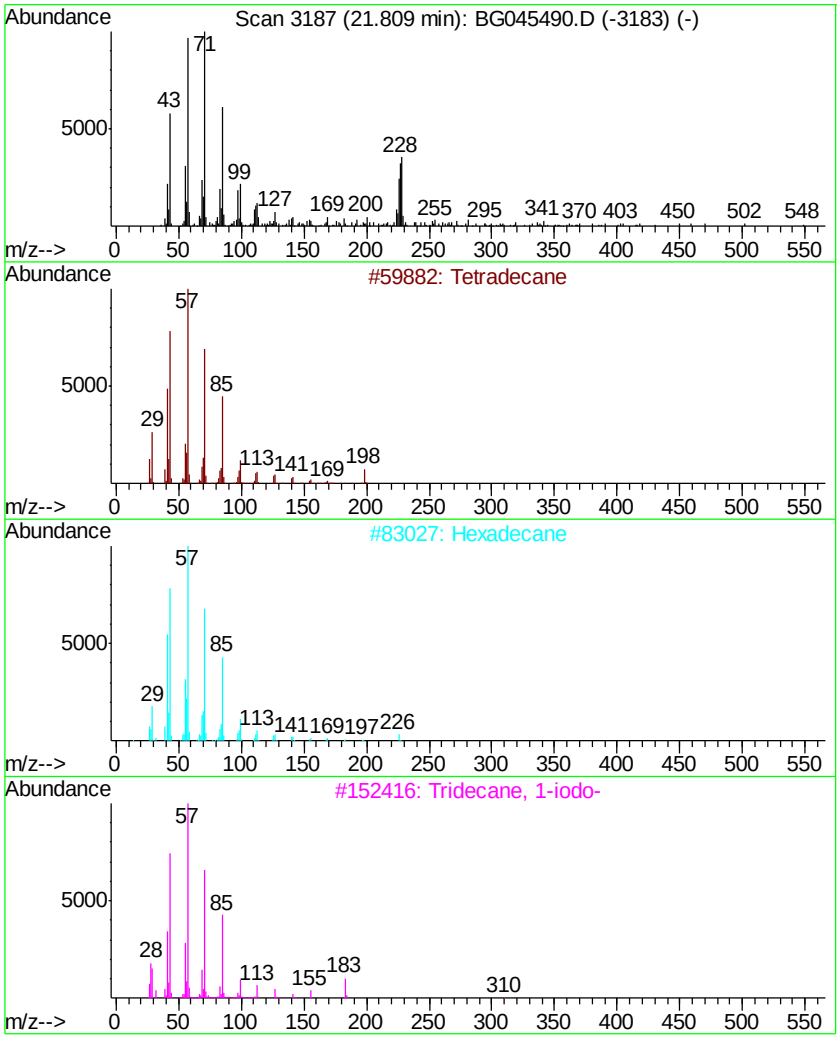
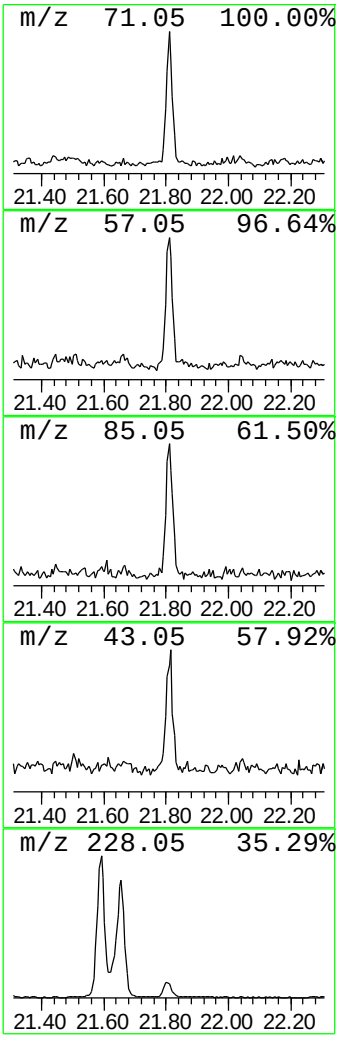
****

Peak Number 5 Tetradecane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.81	2.35 ng	212940	Chrysene-d12	21.61

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetradecane	198	C14H30	000629-59-4	83
2	Hexadecane	226	C16H34	000544-76-3	64
3	Tridecane, 1-iodo-	310	C13H27I	035599-77-0	60
4	Tricosane, 2-methyl-	338	C24H50	001928-30-9	58
5	Hexadecane, 7,9-dimethyl-	254	C18H38	021164-95-4	55





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG052720\
Data File : BG045490.D
Acq On : 28 May 2020 00:23
Operator : CG/JU
Sample : L2745-16
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : NM36-COMP-2020-0-6

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG051520.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

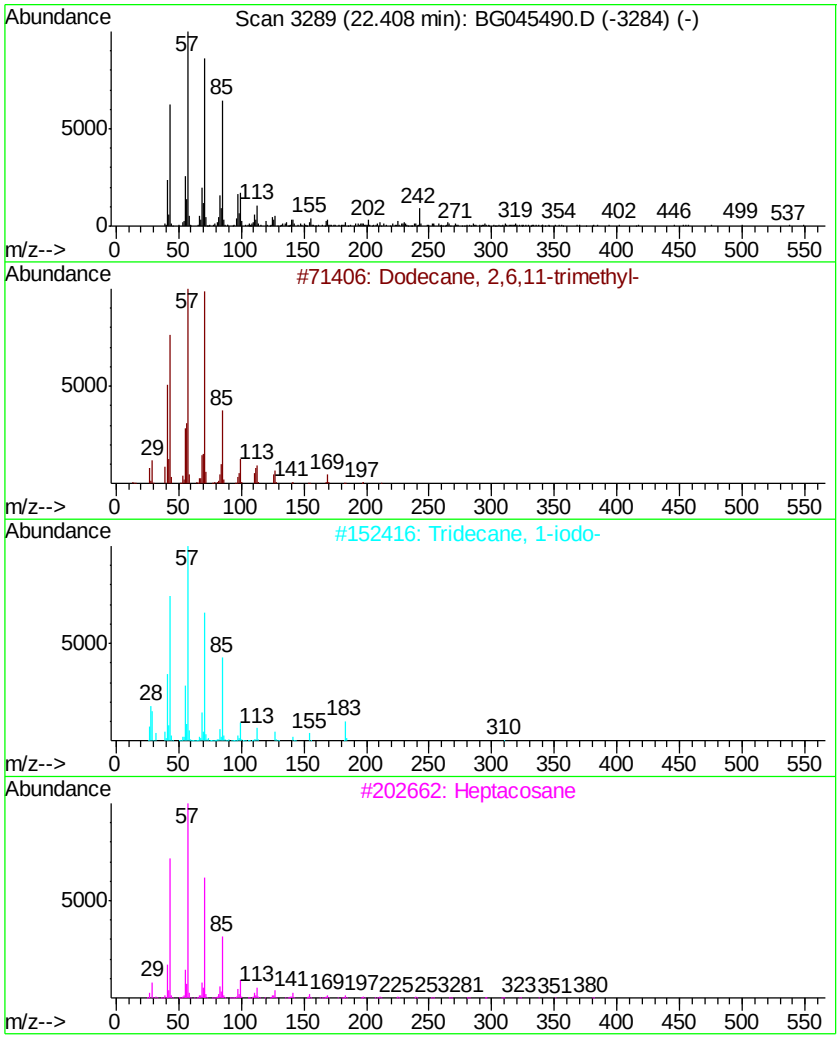
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

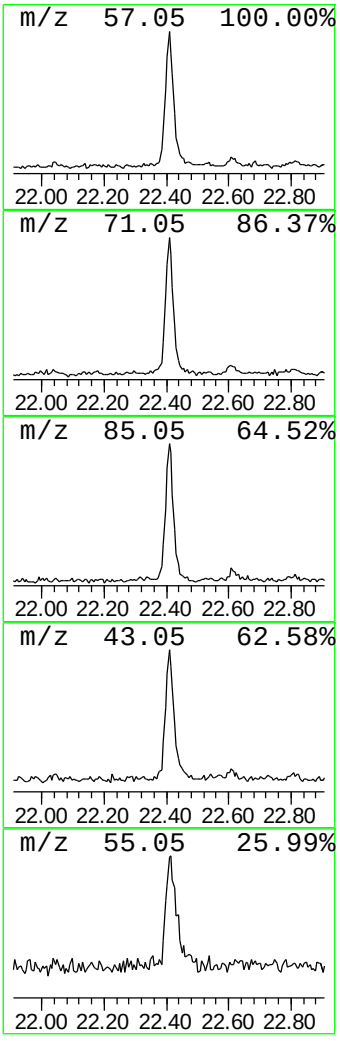
****

Peak Number 6 Dodecane, 2,6,11-trimethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.41	5.20 ng	472038	Chrysene-d12	21.61

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dodecane, 2,6,11-trimethyl-	212	C15H32	031295-56-4	89
2	Tridecane, 1-iodo-	310	C13H27I	035599-77-0	87
3	Heptacosane	380	C27H56	000593-49-7	86
4	Octacosane	394	C28H58	000630-02-4	74
5	Tridecane, 6-propyl-	226	C16H34	055045-10-8	74





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG052720\
Data File : BG045490.D
Acq On : 28 May 2020 00:23
Operator : CG/JU
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Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : NM36-COMP-2020-0-6

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG051520.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
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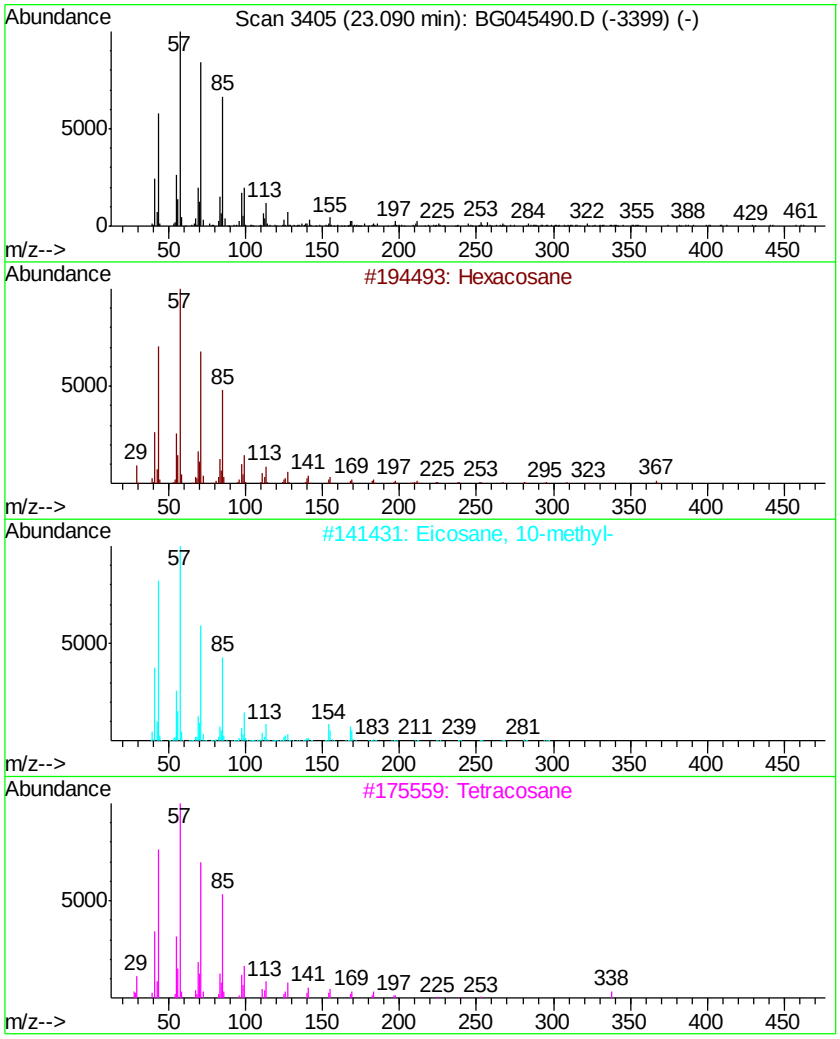
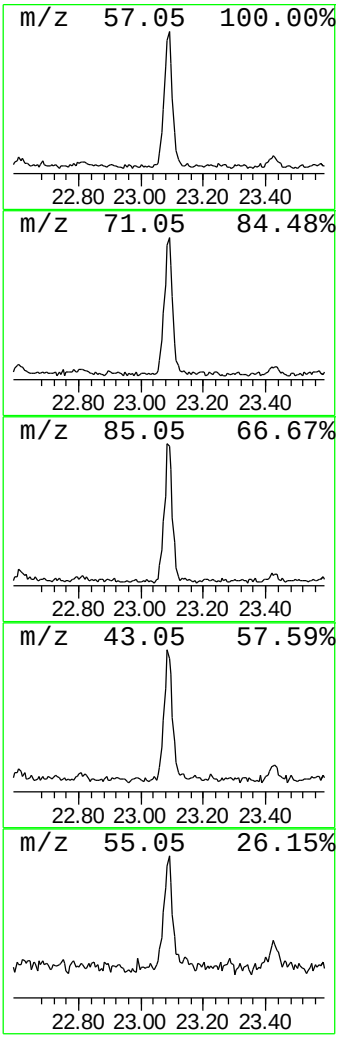
Peak Number 7 Hexacosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.09	4.84 ng	439608	Chrysene-d12	21.61

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosane	366	C26H54	000630-01-3	91
2	Eicosane, 10-methyl-	296	C21H44	054833-23-7	90
3	Tetracosane	338	C24H50	000646-31-1	90
4	Heneicosane	296	C21H44	000629-94-7	87
5	Octacosane	394	C28H58	000630-02-4	80





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Data File : BG045490.D
Acq On : 28 May 2020 00:23
Operator : CG/JU
Sample : L2745-16
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : NM36-COMP-2020-0-6

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG051520.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

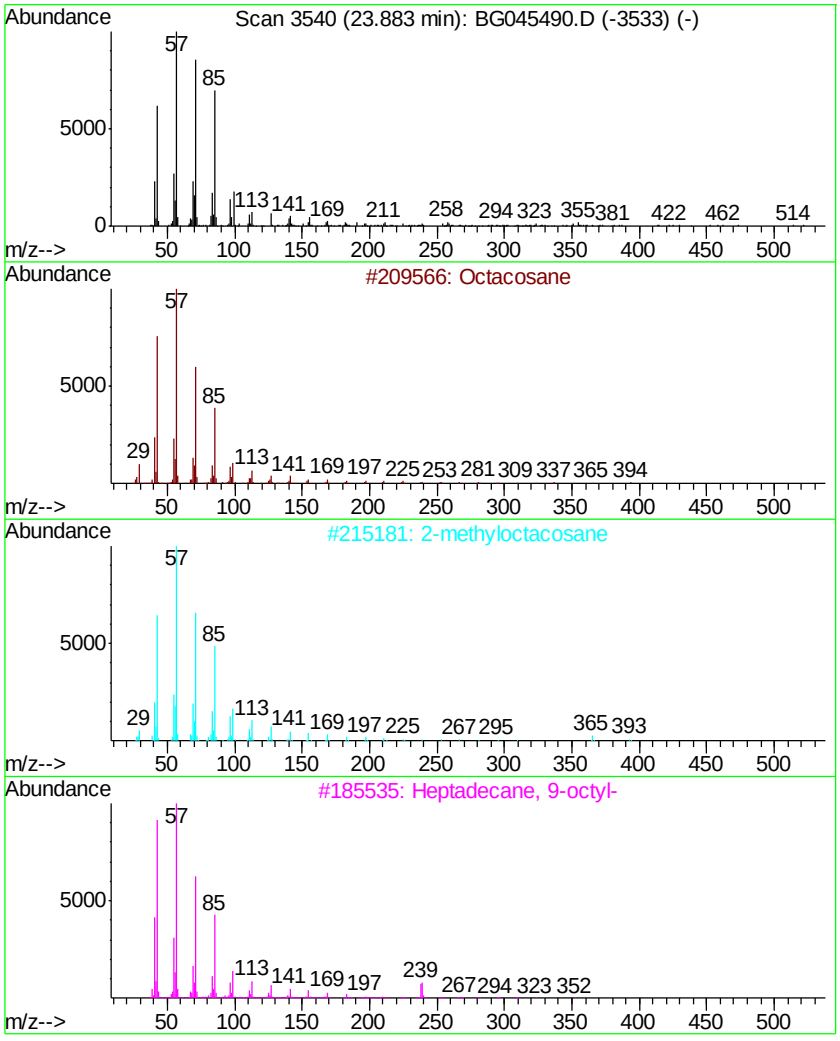
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

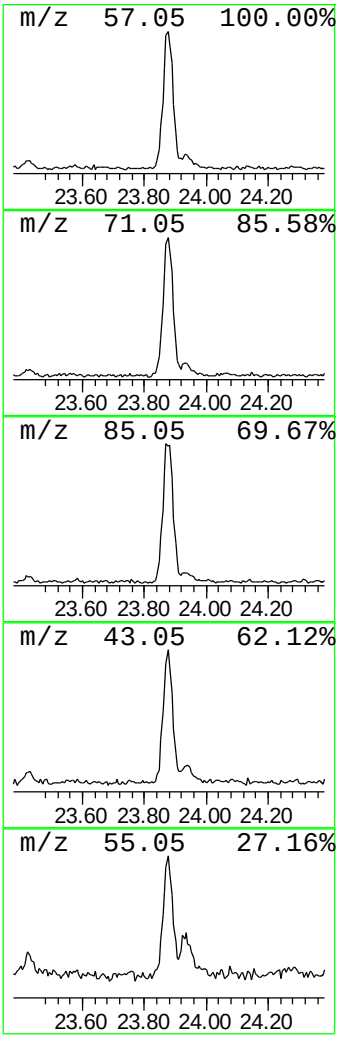
****

Peak Number 8 Octacosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.88	5.98 ng	570644	Perylene-d12	24.76

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane	394	C28H58	000630-02-4	91
2	2-methyloctacosane	408	C29H60	1000376-72-8	90
3	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	87
4	Hexacosane	366	C26H54	000630-01-3	87
5	Tetratetracontane	619	C44H90	007098-22-8	87





Library Search Compound Report

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Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : NM36-COMP-2020-0-6

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG051520.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

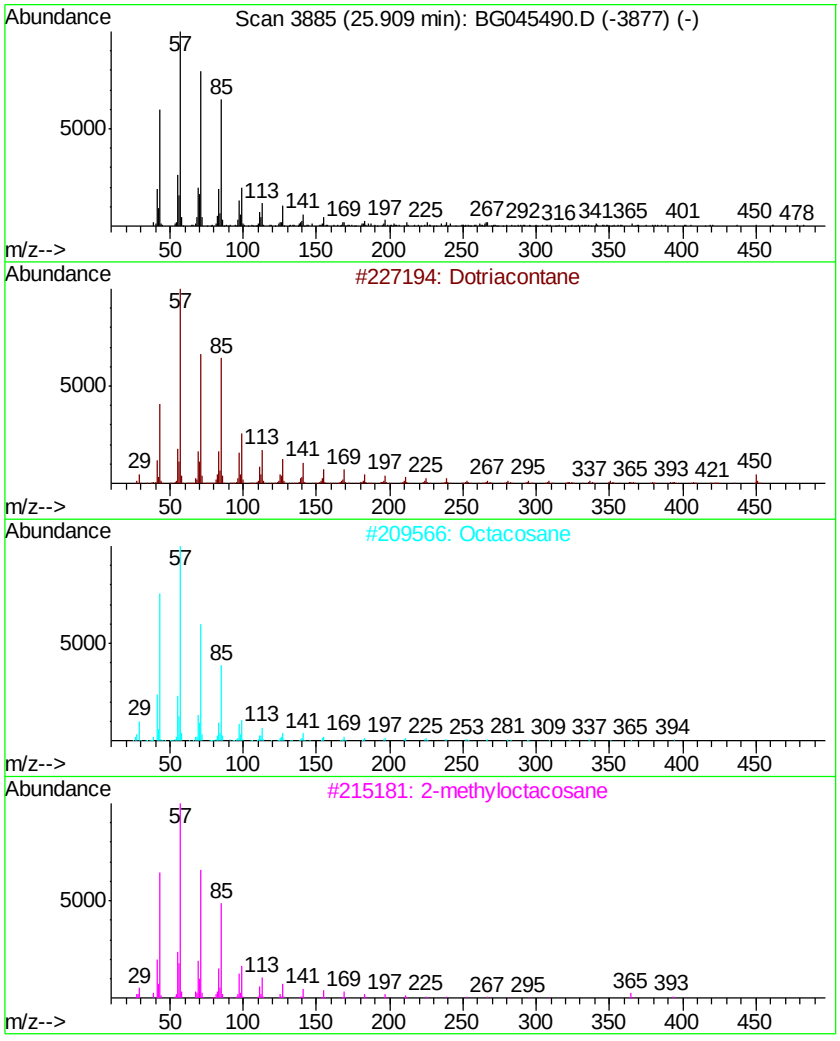
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

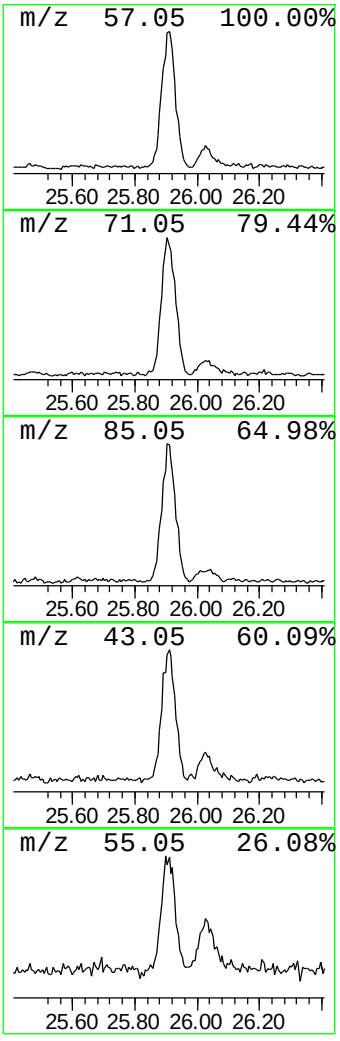
****

Peak Number 9 Dotriacontane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
25.91	8.27 ng	789365	Perylene-d12	24.76

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dotriacontane	451	C32H66	000544-85-4	94
2	Octacosane	394	C28H58	000630-02-4	93
3	2-methyloctacosane	408	C29H60	1000376-72-8	91
4	Hexacosane	366	C26H54	000630-01-3	91
5	Docosane, 11-butyl-	366	C26H54	013475-76-8	91





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG052720\
Data File : BG045490.D
Acq On : 28 May 2020 00:23
Operator : CG/JU
Sample : L2745-16
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : NM36-COMP-2020-0-6

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG051520.M
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
unknown3.12	3.12	6.8	ng	221305	1	7.96	653250	20.0
unknown19.35	19.35	3.3	ng	234752	4	17.35	1446390	20.0
1-Decanol, 2-hexyl-	21.27	4.2	ng	380877	5	21.61	1815470	20.0
Tetradecane	21.81	2.4	ng	212940	5	21.61	1815470	20.0
Dodecane, 2,6,11-...	22.41	5.2	ng	472038	5	21.61	1815470	20.0
Hexacosane	23.09	4.8	ng	439608	5	21.61	1815470	20.0
Octacosane	23.88	6.0	ng	570644	6	24.76	1909280	20.0
Dotriacontane	25.91	8.3	ng	789365	6	24.76	1909280	20.0