LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG051923\
Data File : BG057481.D
Acq On : 20 May 2023 00:23
Operator : CG/JU
Sample : 02849-11
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TP8

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-BG042723.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG057481.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.385	309	314	322	rBB	12978	19655	2.12%	0.403%
2	5.873	391	397	408	rBV	198045	323770	34.88%	6.645%
3	7.494	666	673	684	rBV	210908	373589	40.25%	7.667%
4	8.352	813	819	827	rVB	59454	100584	10.84%	2.064%
5	9.533	1013	1020	1030	rBB	131230	227037	24.46%	4.660%
6	11.189	1294	1302	1311	rBB	77437	140507	15.14%	2.884%
7	13.592	1704	1711	1719	rBV	392046	590400	63.61%	12.117%
8	14.908	1930	1935	1940	rBV2	34477	46420	5.00%	0.953%
9	14.967	1940	1945	1952	rVV	143060	221476	23.86%	4.545%
10	15.190	1980	1983	1989	rVB2	8334	10721	1.16%	0.220%
11	16.306	2168	2173	2179	rVB	30822	43728	4.71%	0.897%
12	16.453	2187	2198	2210	rBV	314433	491065	52.91%	10.078%
13	17.710	2405	2412	2419	rBV	200150	303130	32.66%	6.221%
14	18.550	2550	2555	2564	rBV2	18206	37813	4.07%	0.776%
15	20.277	2843	2849	2858	rBV	726906	928134	100.00%	19.048%
16	21.411	3038	3042	3050	rVB	43021	55233	5.95%	1.134%
17	21.575	3064	3070	3079	rBV4	21453	54241	5.84%	1.113%
18	22.016	3138	3145	3152	rBV	188404	328469	35.39%	6.741%
19	22.791	3273	3277	3281	rBV4	8422	13299	1.43%	0.273%
20	23.537	3399	3404	3410	rVB5	9171	17149	1.85%	0.352%
21	23.743	3436	3439	3444	rBV5	6594	10430	1.12%	0.214%
22	24.401	3542	3551	3558	rBV	32086	71207	7.67%	1.461%
23	25.423	3719	3725	3730	rBV5	11693	27522	2.97%	0.565%
24	25.505	3730	3739	3754	rVB2	108579	323351	34.84%	6.636%
25	26.639	3924	3932	3945	rVB6	26520	81075	8.74%	1.664%
26	28.114	4173	4183	4188	rBV10	9651	32491	3.50%	0.667%

Sum of corrected areas: 4872496

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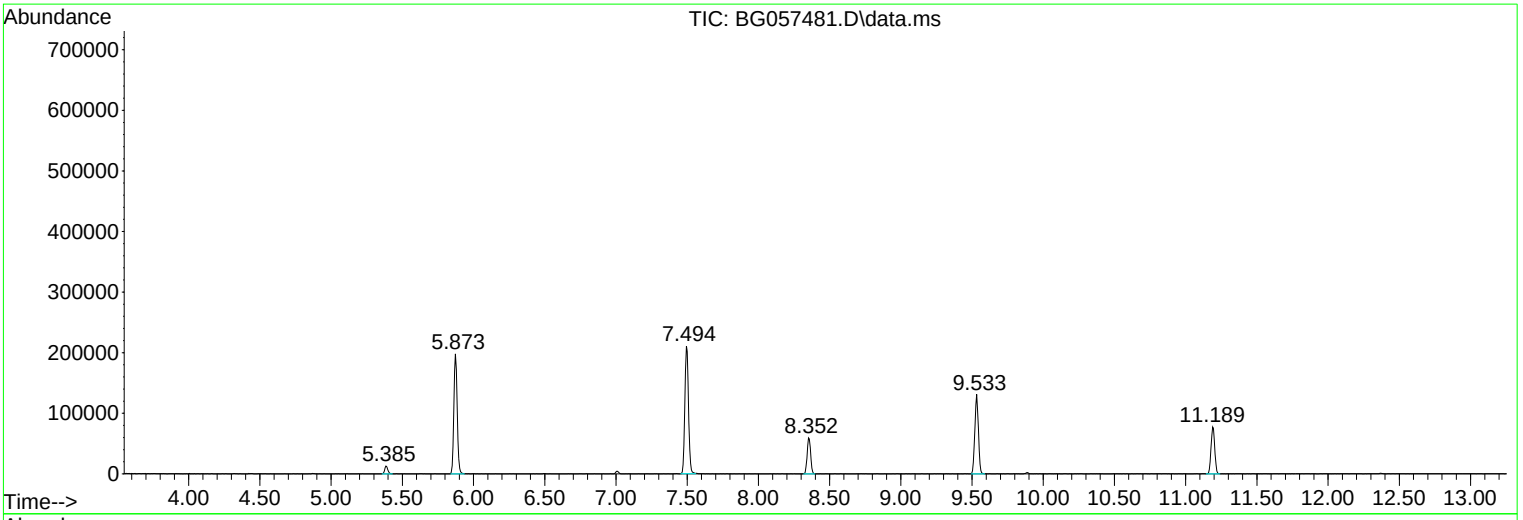
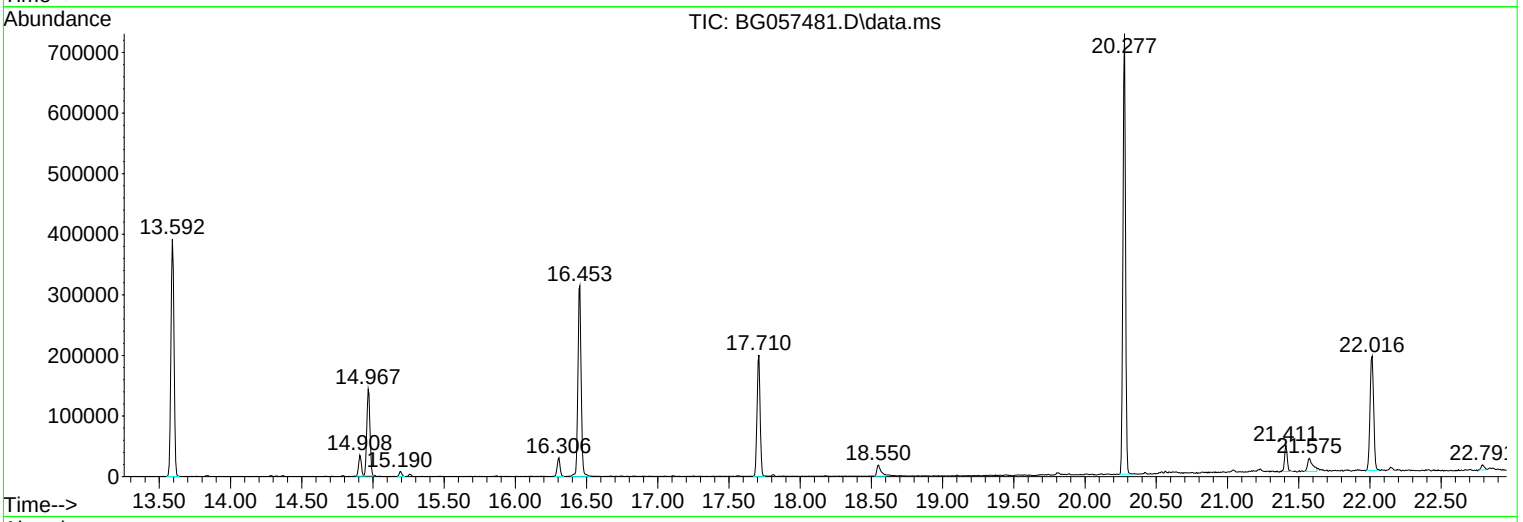
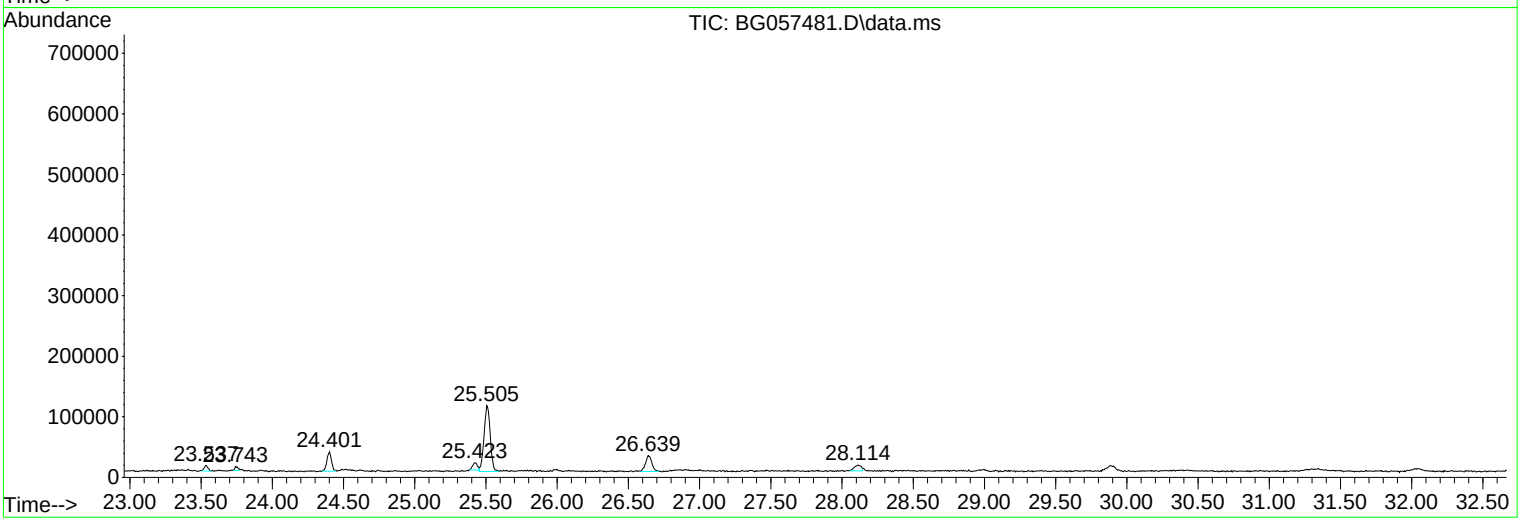
Instrument :
BNA_G
ClientSampleId :
TP8

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG042723.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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TIC Library : C:\Database\NIST20.L
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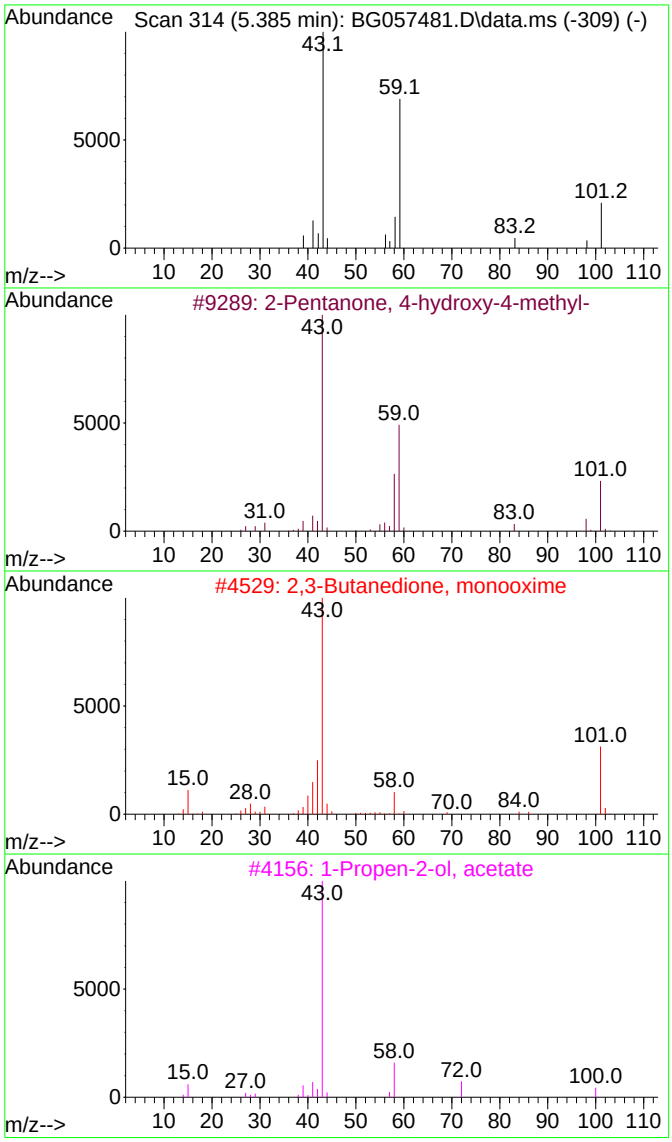
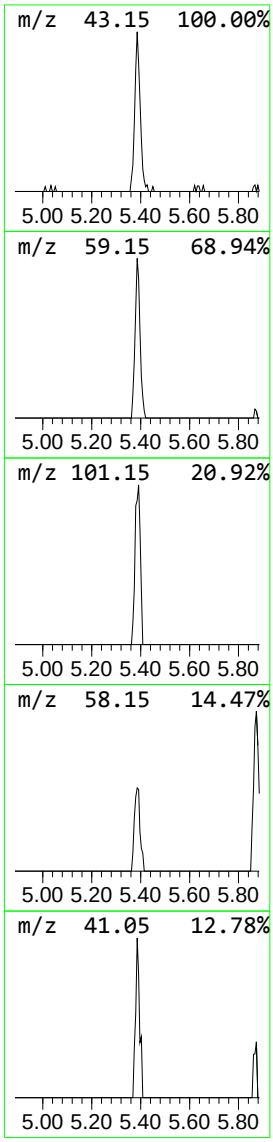
****
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.385	3.91 ng	19655	1,4-Dichlorobenzene-d4	8.352

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
3	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	9
4	Silane, trimethyl-	74	C3H10Si	000993-07-7	9
5	Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	9





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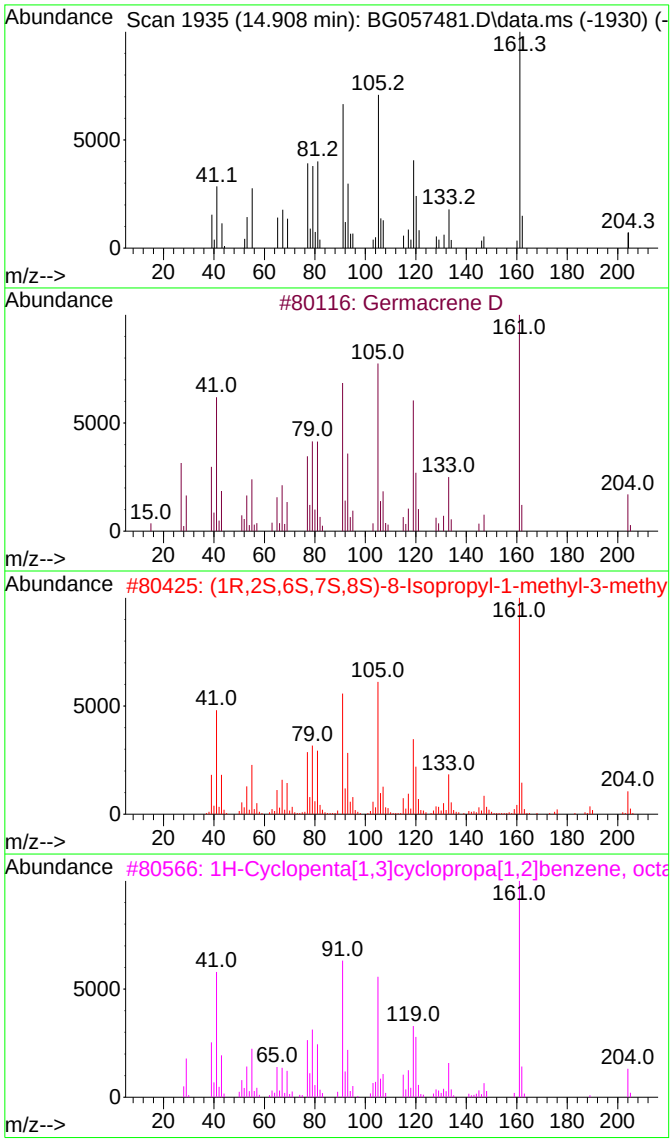
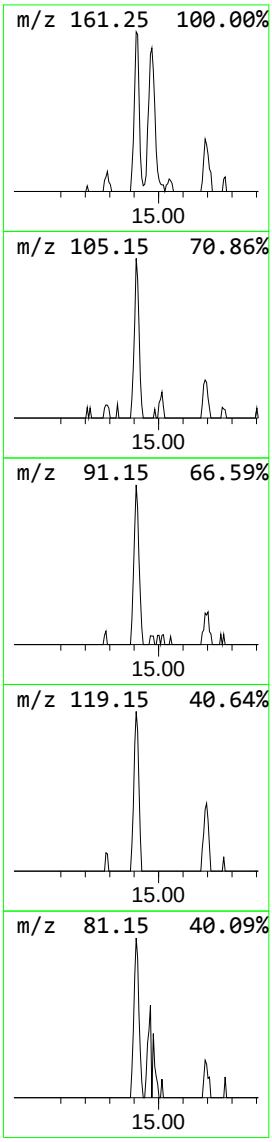
****

Peak Number 2 Germacrene D Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.908	4.19 ng	46420	Acenaphthene-d10	14.967

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Germacrene D	204	C15H24	023986-74-5	99
2	(1R,2S,6S,7S,8S)-8-Isopropyl-1-m...	204	C15H24	018252-44-3	94
3	1H-Cyclopenta[1,3]cyclopropa[1,2...	204	C15H24	013744-15-5	93
4	(+)-epi-Bicyclosesquiphellandrene	204	C15H24	054274-73-6	93
5	.alpha.-Cubebene	204	C15H24	017699-14-8	91





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Instrument :
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ClientSampleId :
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TIC Library : C:\Database\NIST20.L
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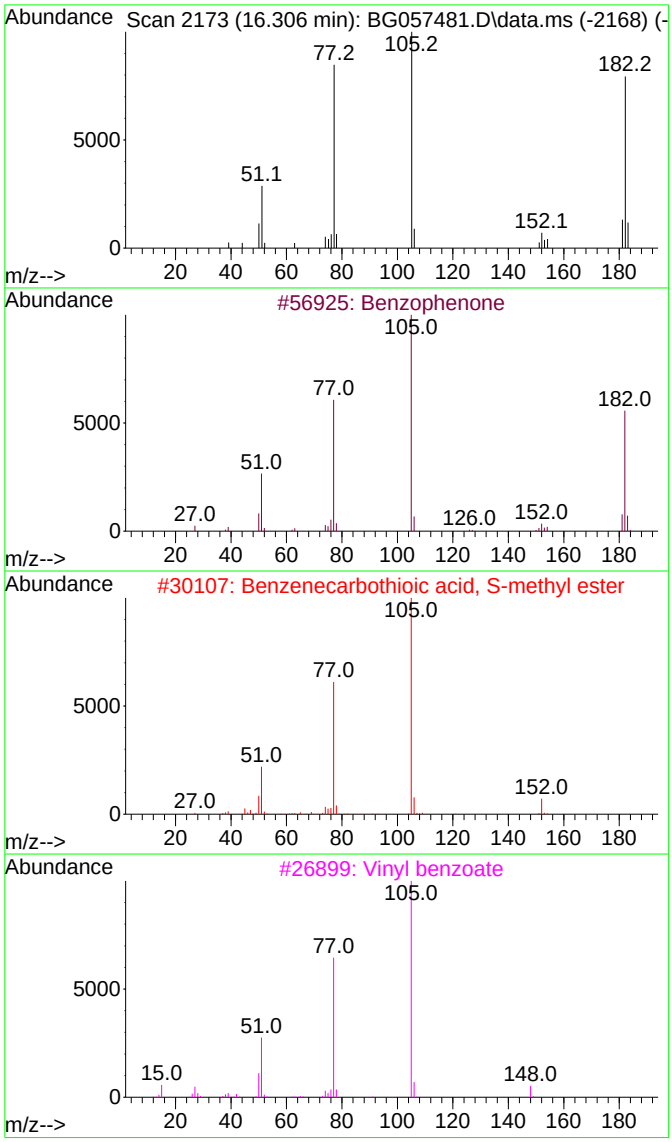
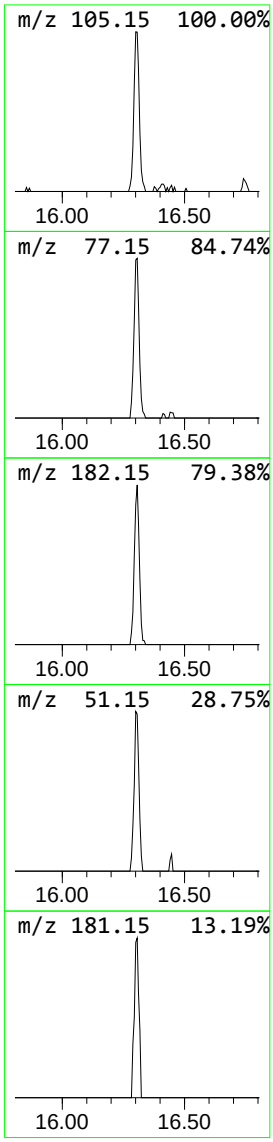
Peak Number 3 Benzophenone Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.306	3.95 ng	43728	Acenaphthene-d10	14.967

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	97
2	Benzenecarbothioic acid, S-methy...	152	C8H8OS	005925-68-8	46
3	Vinyl benzoate	148	C9H8O2	000769-78-8	38
4	Ethanone, 2,2,2-trifluoro-1-phenyl-	174	C8H5F3O	000434-45-7	38
5	1,2-Propanedione, 1-phenyl-	148	C9H8O2	000579-07-7	38





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Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG042723.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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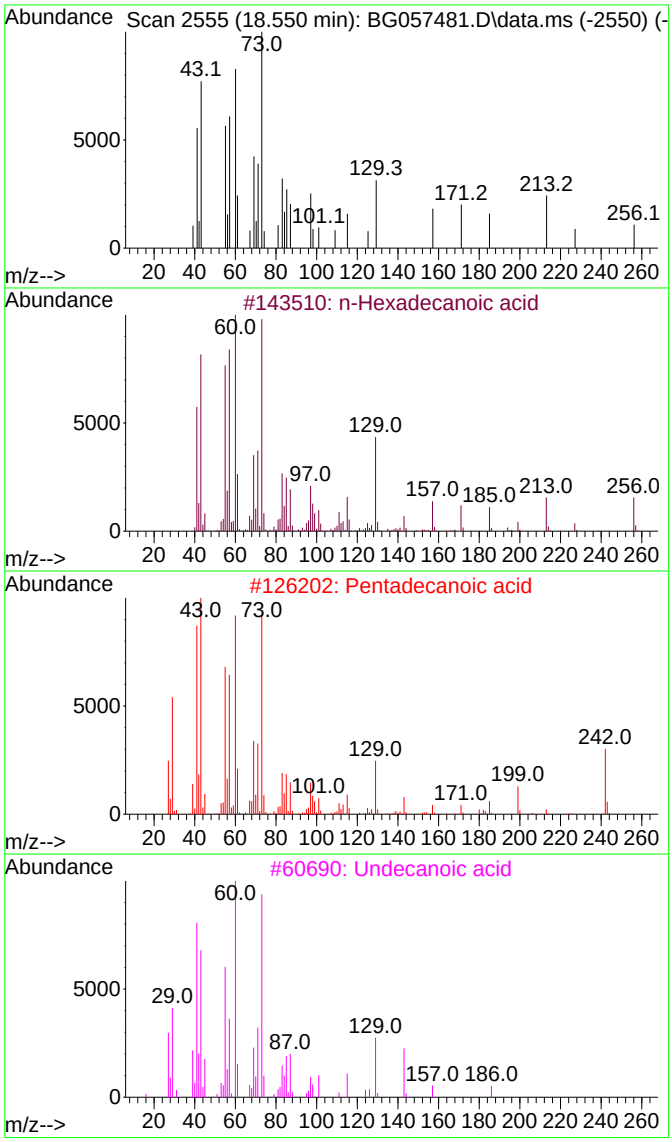
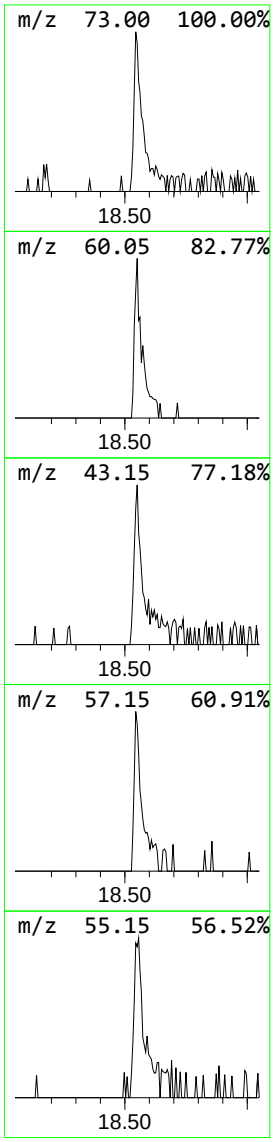
Peak Number 4 n-Hexadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.550	2.49 ng	37813	Phenanthrene-d10	17.710

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	95
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	72
3	Undecanoic acid	186	C11H22O2	000112-37-8	53
4	Dodecanoic acid	200	C12H24O2	000143-07-7	50
5	.beta.-D-Mannofuranoside, 1-O-(1...	332	C17H32O6	1000155-29-9	14





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Sample : 02849-11
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
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TIC Library : C:\Database\NIST20.L
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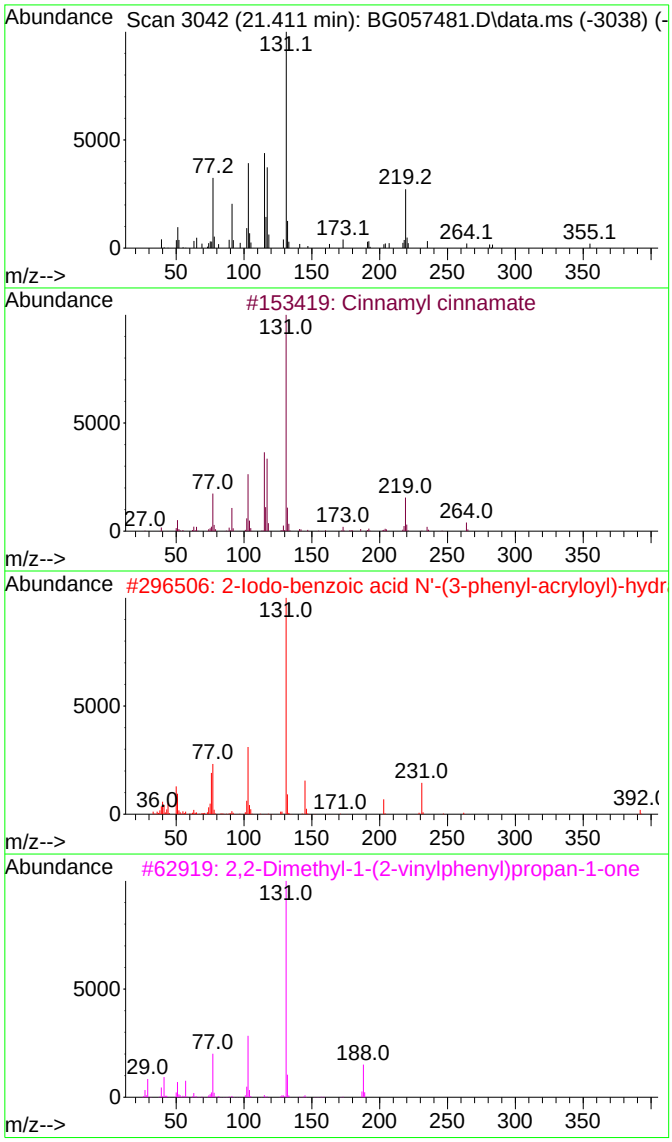
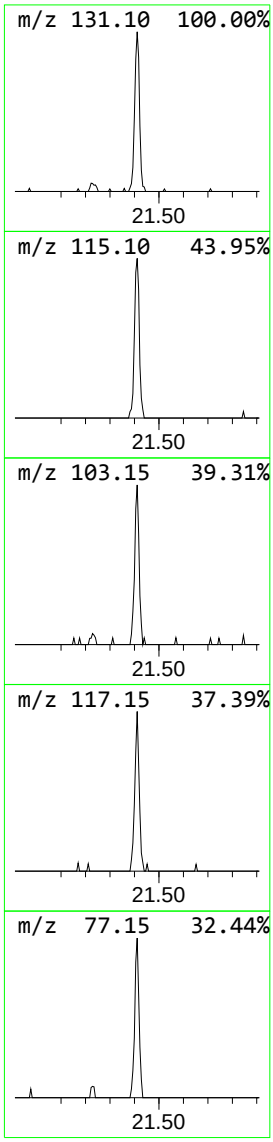
Peak Number 5 Cinnamyl cinnamate Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.411	3.36 ng	55233	Chrysene-d12	22.010

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cinnamyl cinnamate	264	C18H16O2	000122-69-0	91
2	2-Iodo-benzoic acid N'-(3-phenyl...	392	C16H13IN2O2	315672-62-9	47
3	2,2-Dimethyl-1-(2-vinylphenyl)pr...	188	C13H16O	1000210-99-9	47
4	3-phenylprop-2-enoic anhydride	278	C18H14O3	1010401-87-5	47
5	2-Propenoic acid, 3-phenyl-, 4-m...	238	C16H14O2	010519-07-0	47





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Sample : 02849-11
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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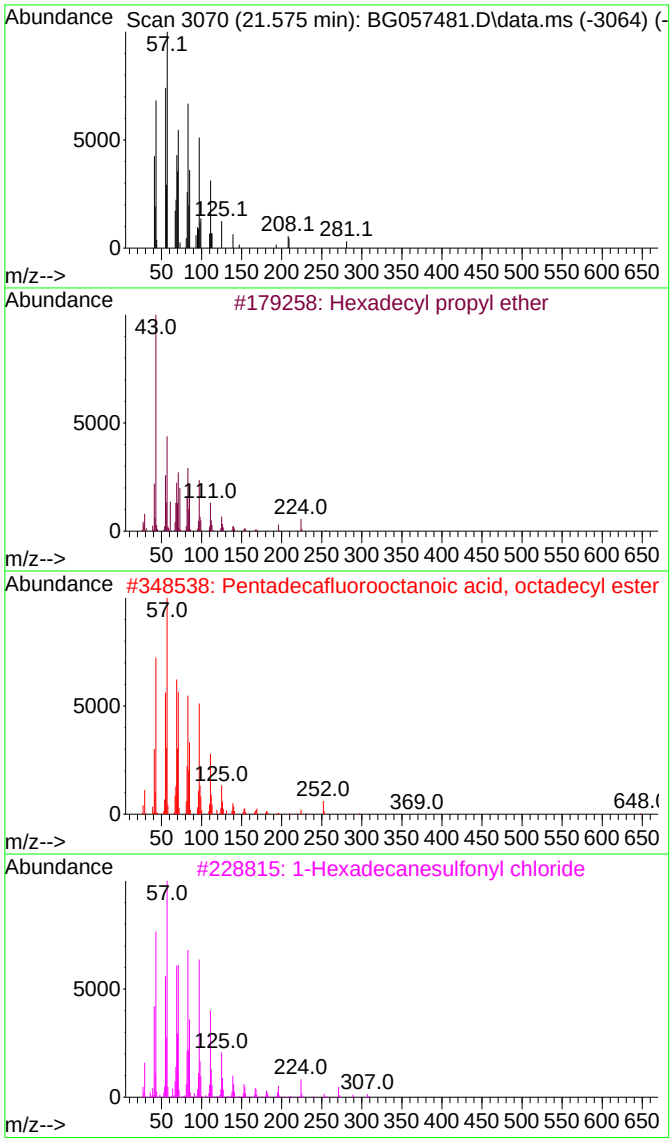
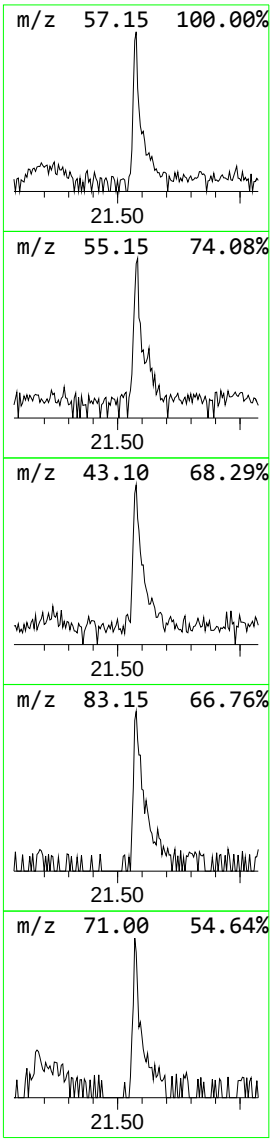
Peak Number 6 Hexadecyl propyl ether Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.575	3.30 ng	54241	Chrysene-d12	22.010

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecyl propyl ether	284	C19H40O	1000406-27-9	91
2	Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	91
3	1-Hexadecanesulfonyl chloride	324	C16H33ClO2S	038775-38-1	91
4	17-Pentatriacontene	491	C35H70	006971-40-0	91
5	2- Bromopropionic acid, pentadec...	362	C18H35BrO2	1000292-44-2	87





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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG042723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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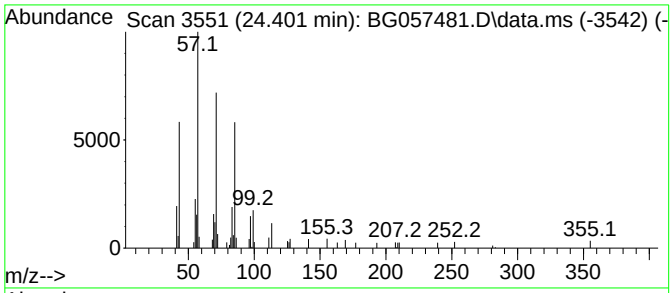
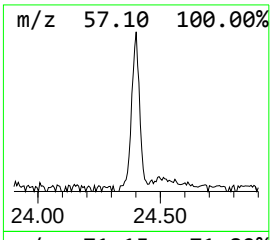
****

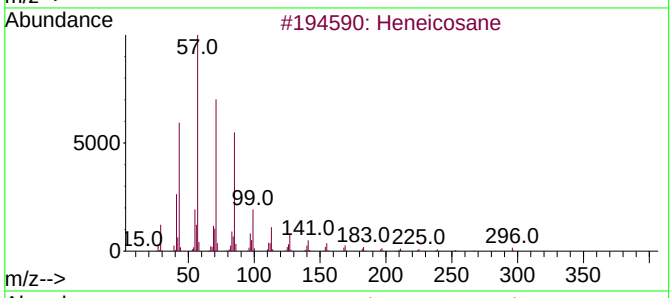
Peak Number 7 Heneicosane Concentration Rank 2

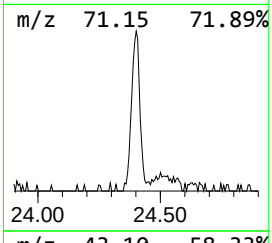
R.T.	EstConc	Area	Relative to ISTD	R.T.
24.401	4.40 ng	71207	Perylene-d12	25.505

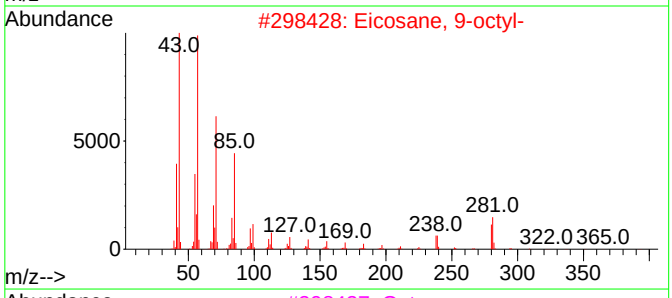
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	86
2	Eicosane, 9-octyl-	394	C28H58	013475-77-9	86
3	Octacosane	394	C28H58	000630-02-4	86
4	Tridecane, 1-iodo-	310	C13H27I	035599-77-0	80
5	Heptadecane	240	C17H36	000629-78-7	80

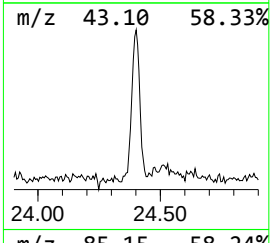


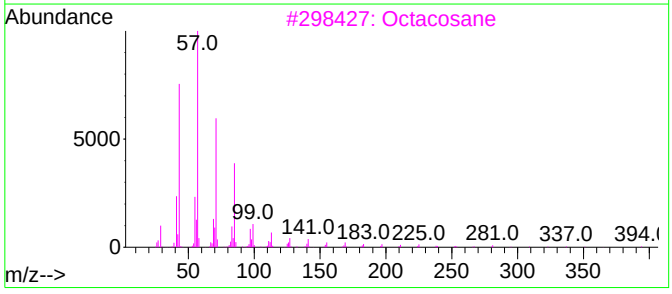


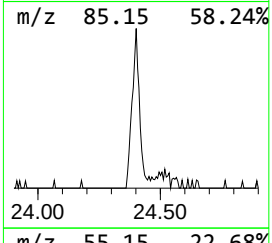


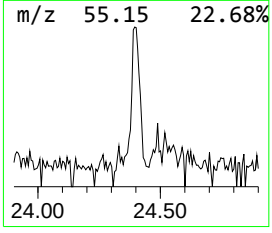












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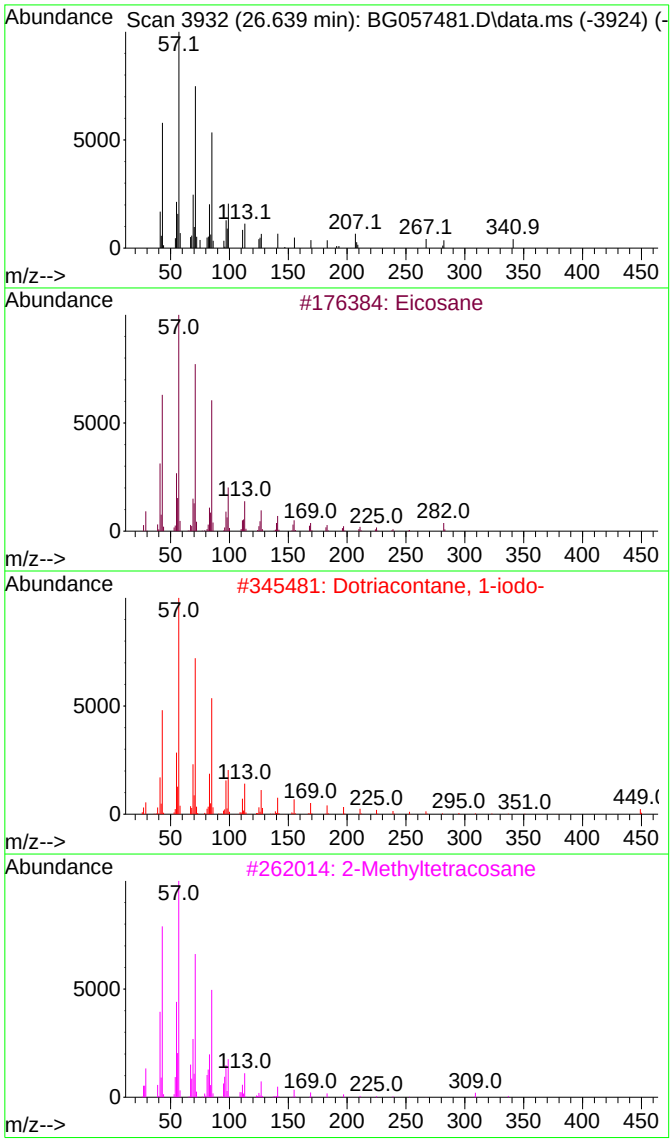
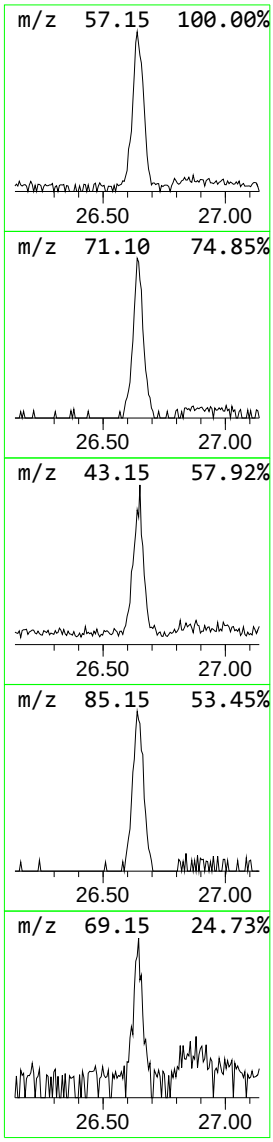
****

Peak Number 8 Eicosane Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
26.639	5.01 ng	81075	Perylene-d12	25.505

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	97
2	Dotriacontane, 1-iodo-	576	C32H65I	1000406-32-4	91
3	2-Methyltetracosane	352	C25H52	001560-78-7	90
4	Pentadecane, 7-(bromomethyl)-	304	C16H33Br	052997-43-0	90
5	2-Methylhexacosane	380	C27H56	001561-02-0	90





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG051923\
Data File : BG057481.D
Acq On : 20 May 2023 00:23
Operator : CG/JU
Sample : 02849-11
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TP8

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG042723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

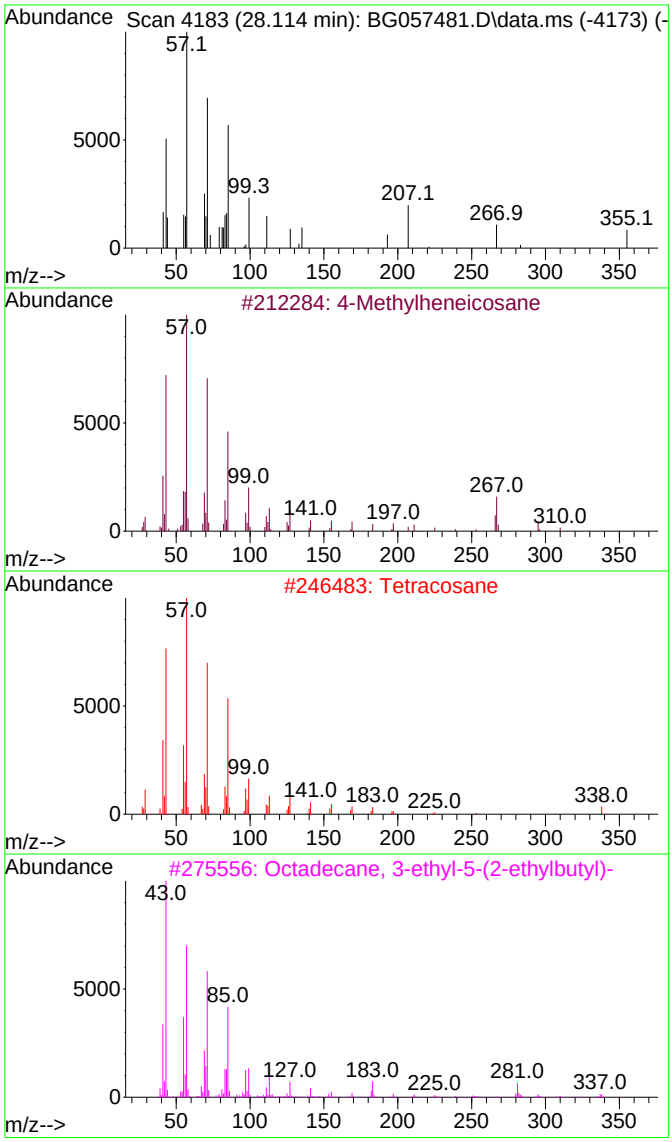
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

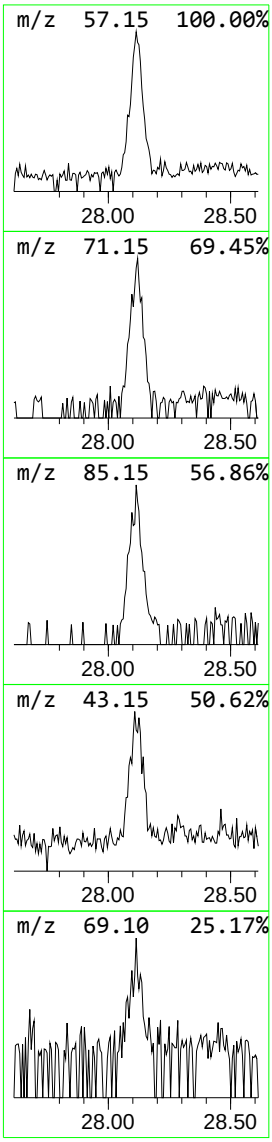
****

Peak Number 9 4-Methylheneicosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
28.114	2.01 ng	32491	Perylene-d12	25.505

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Methylheneicosane	310	C22H46	025117-29-7	59
2	Tetracosane	338	C24H50	000646-31-1	53
3	Octadecane, 3-ethyl-5-(2-ethylbu...	366	C26H54	055282-12-7	53
4	Pentadecane, 7-(bromomethyl)-	304	C16H33Br	052997-43-0	53
5	Heptadecane	240	C17H36	000629-78-7	53





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG051923\
Data File : BG057481.D
Acq On : 20 May 2023 00:23
Operator : CG/JU
Sample : 02849-11
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TP8

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG042723.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-...	5.385	3.9	ng	19655	1	8.352	100584	20.0
Germacrene D	14.908	4.2	ng	46420	3	14.967	221476	20.0
Benzophenone	16.306	4.0	ng	43728	3	14.967	221476	20.0
n-Hexadecanoic ...	18.550	2.5	ng	37813	4	17.710	303130	20.0
Cinnamyl cinnamate	21.411	3.4	ng	55233	5	22.010	328469	20.0
Hexadecyl propy...	21.575	3.3	ng	54241	5	22.010	328469	20.0
Heneicosane	24.401	4.4	ng	71207	6	25.505	323351	20.0
Eicosane	26.639	5.0	ng	81075	6	25.505	323351	20.0
4-Methylheneico...	28.114	2.0	ng	32491	6	25.505	323351	20.0