LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG060120\
Data File : BG045566.D
Acq On : 1 Jun 2020 21:57
Operator : CG/JU
Sample : L2792-08
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : NM114-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	5.544	411	418	433	rBV	793837	1351433	40.41%	4.964%
2	7.154	683	692	705	rBV	876955	1562949	46.73%	5.741%
3	7.953	821	828	836	rBV	282985	485978	14.53%	1.785%
4	8.276	875	883	892	rBV	778964	1392306	41.63%	5.114%
5	9.116	1018	1026	1037	rBV	582571	1084329	32.42%	3.983%
6	10.761	1297	1306	1322	rBV	365655	704175	21.06%	2.586%
7	13.216	1716	1724	1740	rBV	1658037	2697733	80.67%	9.909%
8	13.839	1822	1830	1836	rBV3	50299	81677	2.44%	0.300%
9	14.044	1859	1865	1871	rBV	243934	364711	10.91%	1.340%
10	14.444	1922	1933	1939	rBV3	81951	127686	3.82%	0.469%
11	14.514	1939	1945	1949	rVB4	22831	34475	1.03%	0.127%
12	14.597	1949	1959	1966	rBV	631177	1026768	30.70%	3.771%
13	16.089	2206	2213	2223	rBV	1268678	1990015	59.50%	7.309%
14	16.747	2319	2325	2330	rBV7	24812	55274	1.65%	0.203%
15	17.346	2417	2427	2431	rBV	706739	1100178	32.90%	4.041%
16	17.387	2431	2434	2440	rVB	115922	171889	5.14%	0.631%
17	17.722	2487	2491	2494	rBV5	28968	43833	1.31%	0.161%
18	17.874	2514	2517	2522	rVB6	21963	35450	1.06%	0.130%
19	18.192	2567	2571	2574	rBV6	30773	41428	1.24%	0.152%
20	18.250	2578	2581	2589	rVB4	61818	126485	3.78%	0.465%
21	18.415	2605	2609	2614	rBV3	35124	65323	1.95%	0.240%
22	18.761	2664	2668	2675	rVB9	19051	40695	1.22%	0.149%
23	19.267	2749	2754	2760	rBV6	37902	82281	2.46%	0.302%
24	19.343	2762	2767	2772	rVV	344833	489315	14.63%	1.797%
25	19.396	2772	2776	2783	rVB	328066	476952	14.26%	1.752%
26	19.760	2829	2838	2845	rBV	300921	522393	15.62%	1.919%
27	19.960	2866	2872	2878	rBV	2497619	3344358	100.00%	12.284%
28	20.248	2917	2921	2927	rVB3	60491	123728	3.70%	0.454%
29	20.600	2978	2981	2985	rBV5	49959	66094	1.98%	0.243%
30	21.258	3090	3093	3101	rVB4	221812	372747	11.15%	1.369%
31	21.605	3144	3152	3157	rBV2	675205	1342057	40.13%	4.929%
32	21.652	3157	3160	3168	rVB	132405	208961	6.25%	0.768%
33	21.799	3183	3185	3192	rVB7	51482	86954	2.60%	0.319%
34	22.415	3285	3290	3298	rVB5	130672	314283	9.40%	1.154%

LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG060120\
Data File : BG045566.D
Acq On : 1 Jun 2020 21:57
Operator : CG/JU
Sample : L2792-08
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : NM114-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	23.420	3455	3461	3468	rVB2	260945	512383	15.32%	1.882%
36	23.761	3513	3519	3526	rBV	103838	289914	8.67%	1.065%
37	23.872	3533	3538	3542	rBV2	136522	234522	7.01%	0.861%
38	23.925	3542	3547	3558	rVB3	397225	931810	27.86%	3.423%
39	24.747	3679	3687	3698	rBV	372048	1118425	33.44%	4.108%
40	25.300	3774	3781	3789	rVB4	146222	392929	11.75%	1.443%
41	25.899	3874	3883	3894	rVB2	410328	1215423	36.34%	4.464%
42	26.016	3897	3903	3916	rVB3	161876	514822	15.39%	1.891%

Sum of corrected areas: 27225141

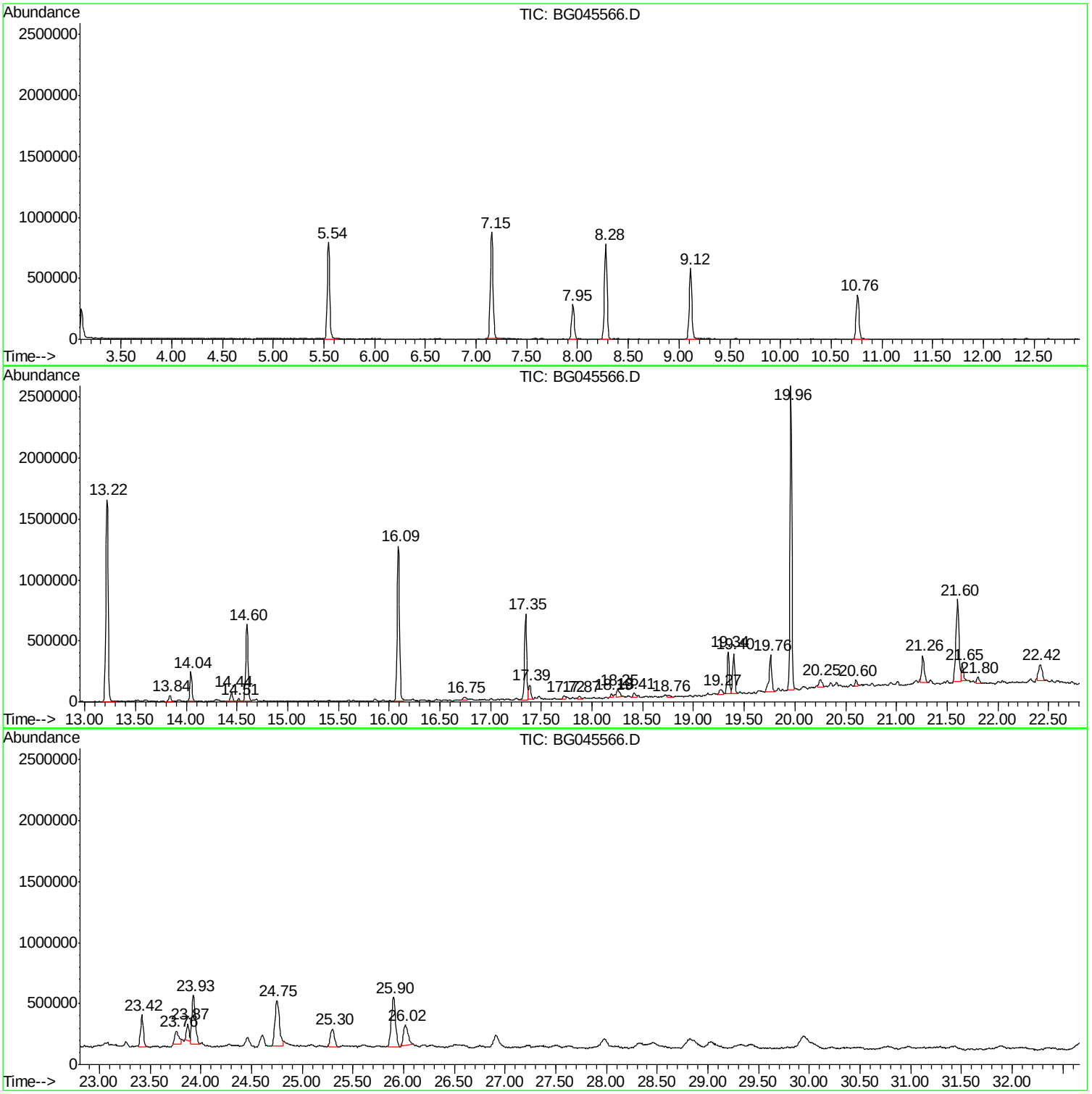
LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG060120\
Data File : BG045566.D
Acq On : 1 Jun 2020 21:57
Operator : CG/JU
Sample : L2792-08
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
NM114-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



Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG060120\
Data File : BG045566.D
Acq On : 1 Jun 2020 21:57
Operator : CG/JU
Sample : L2792-08
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : NM114-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

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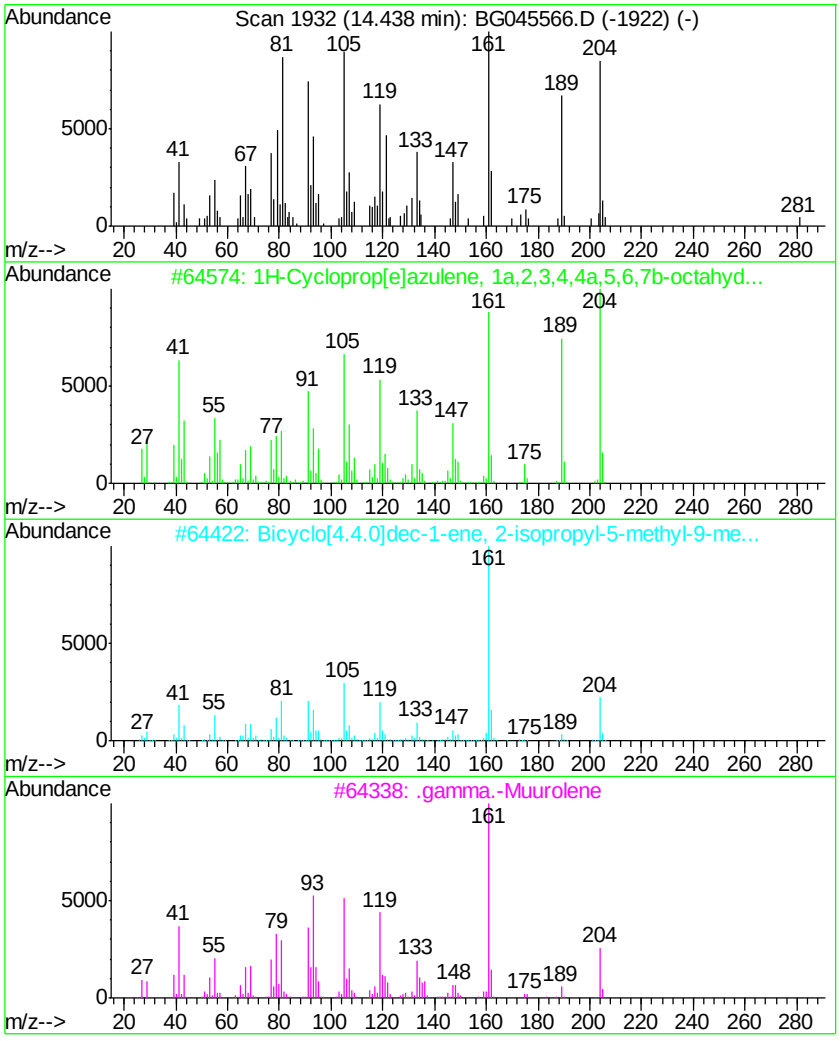
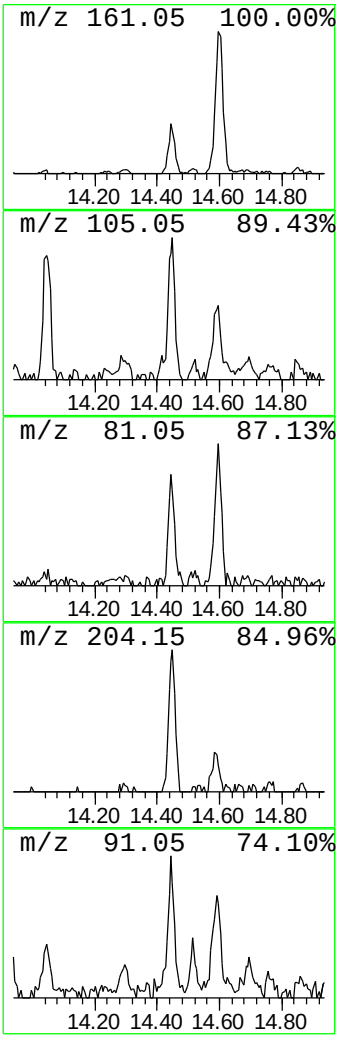
Peak Number 2 1H-Cycloprop[e]azulene, 1a,... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.44	2.49 ng	127686	Acenaphthene-d10	14.60

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Cycloprop[e]azulene, 1a,2,3,4...	204	C15H24	000489-40-7	95
2	Bicyclo[4.4.0]dec-1-ene, 2-isopr...	204	C15H24	150320-52-8	83
3	.gamma.-Muurolene	204	C15H24	030021-74-0	83
4	cis-muurola-3,5-diene	204	C15H24	1000365-95-4	83
5	Cyclohexene, 6-ethenyl-6-methyl-...	204	C15H24	005951-67-7	83





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG060120\
Data File : BG045566.D
Acq On : 1 Jun 2020 21:57
Operator : CG/JU
Sample : L2792-08
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : NM114-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

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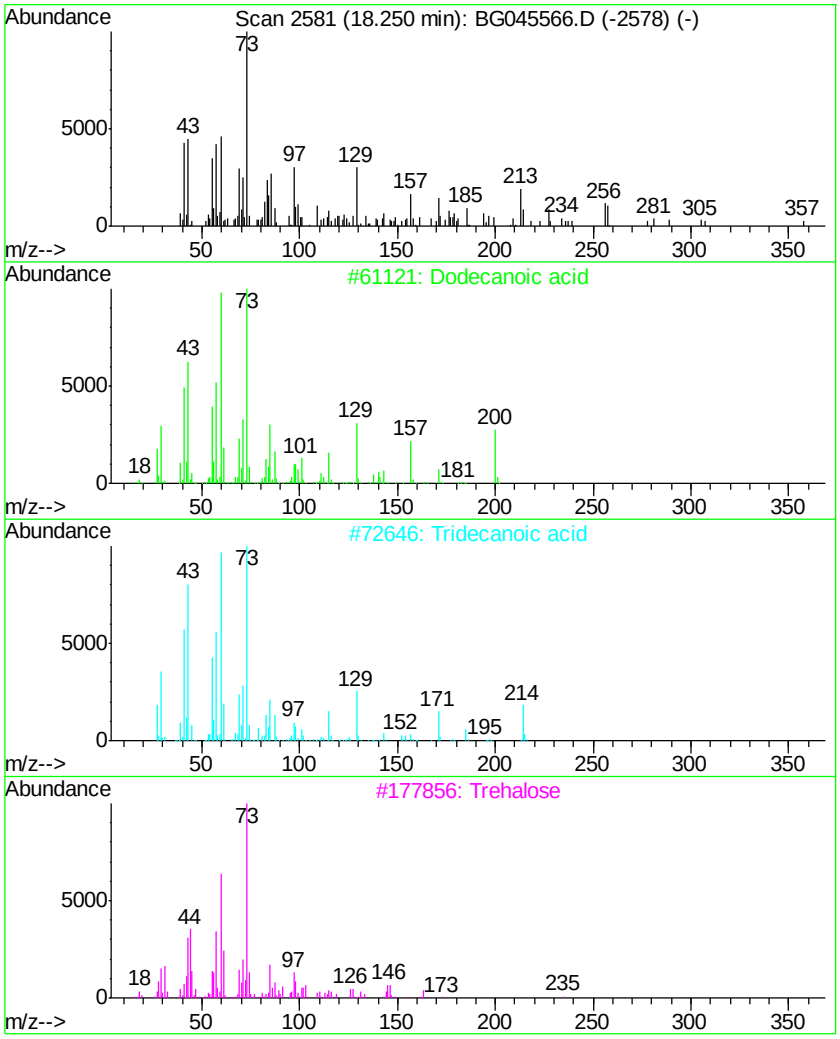
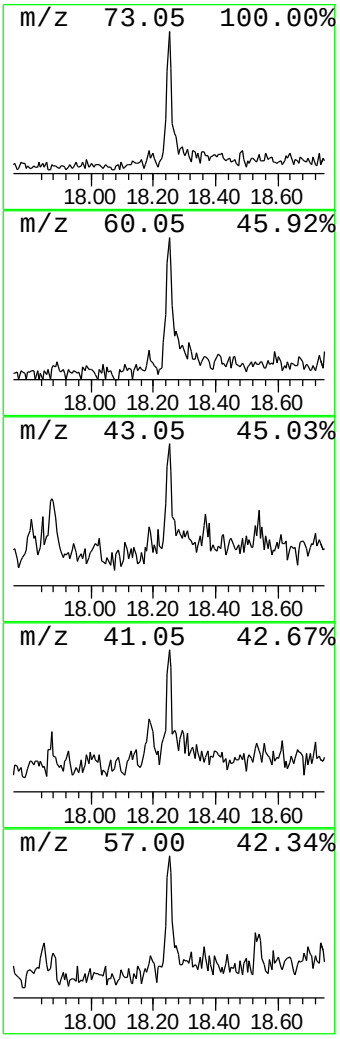
Peak Number 3 unknown18.25 Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.25	2.30 ng	126485	Phenanthrene-d10	17.35

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dodecanoic acid	200	C12H24O2	000143-07-7	37
2	Tridecanoic acid	214	C13H26O2	000638-53-9	35
3	Trehalose	342	C12H22O11	000099-20-7	32
4	Octadecanoic acid	284	C18H36O2	000057-11-4	32
5	Pentadecanoic acid	242	C15H30O2	001002-84-2	25





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG060120\
Data File : BG045566.D
Acq On : 1 Jun 2020 21:57
Operator : CG/JU
Sample : L2792-08
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : NM114-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

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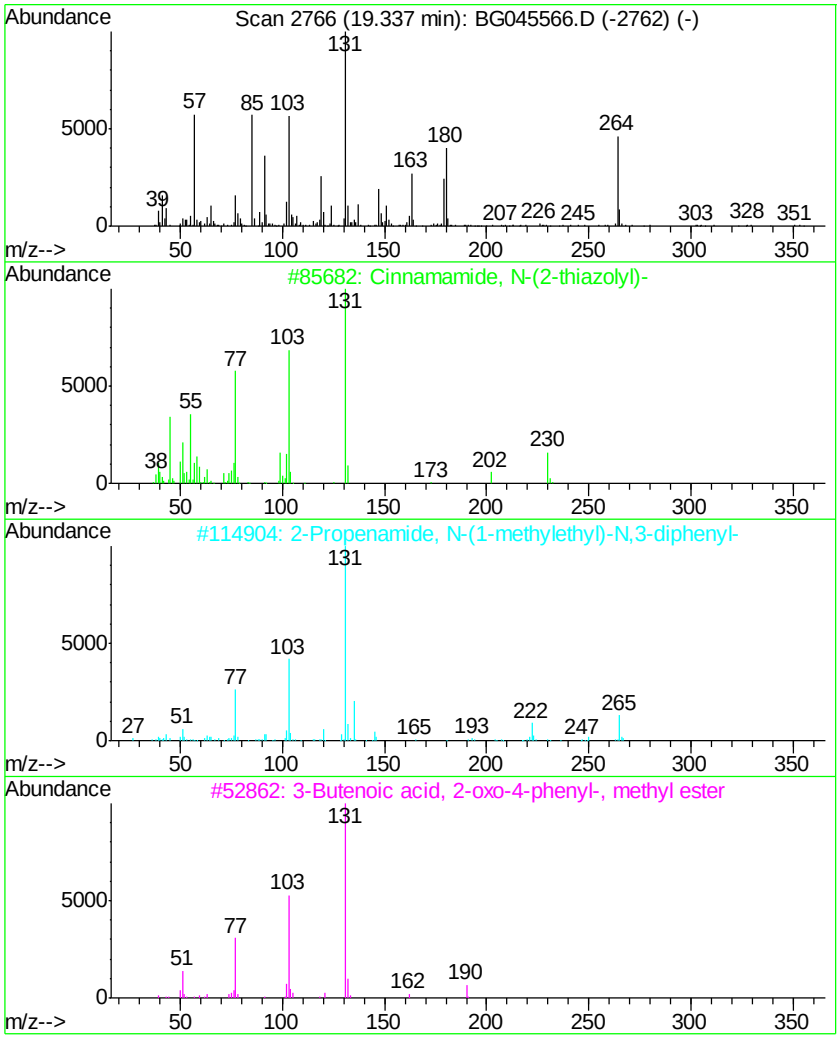
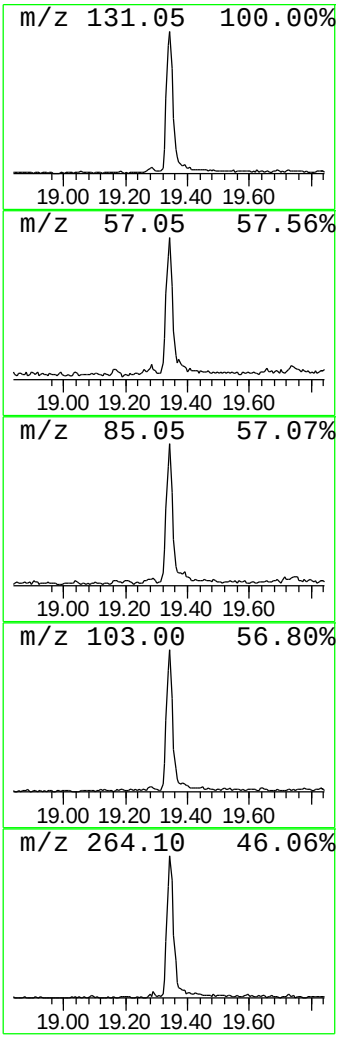
Peak Number 4 unknown19.34 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.34	8.90 ng	489315	Phenanthrene-d10	17.35

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cinnamamide, N-(2-thiazolyl)-	230	C12H10N2OS	300829-00-9	27
2	2-Propenamide, N-(1-methylethyl)...	265	C18H19NO	055044-37-6	27
3	3-Butenoic acid, 2-oxo-4-phenyl-...	190	C11H10O3	1000142-22-4	27
4	Silane, ethoxytriethyl-	160	C8H20OSi	000597-67-1	27
5	7-Oxo-1,3,5-cycloheptatriene-1-c...	131	C8H5NO	000934-19-0	16





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG060120\
Data File : BG045566.D
Acq On : 1 Jun 2020 21:57
Operator : CG/JU
Sample : L2792-08
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : NM114-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

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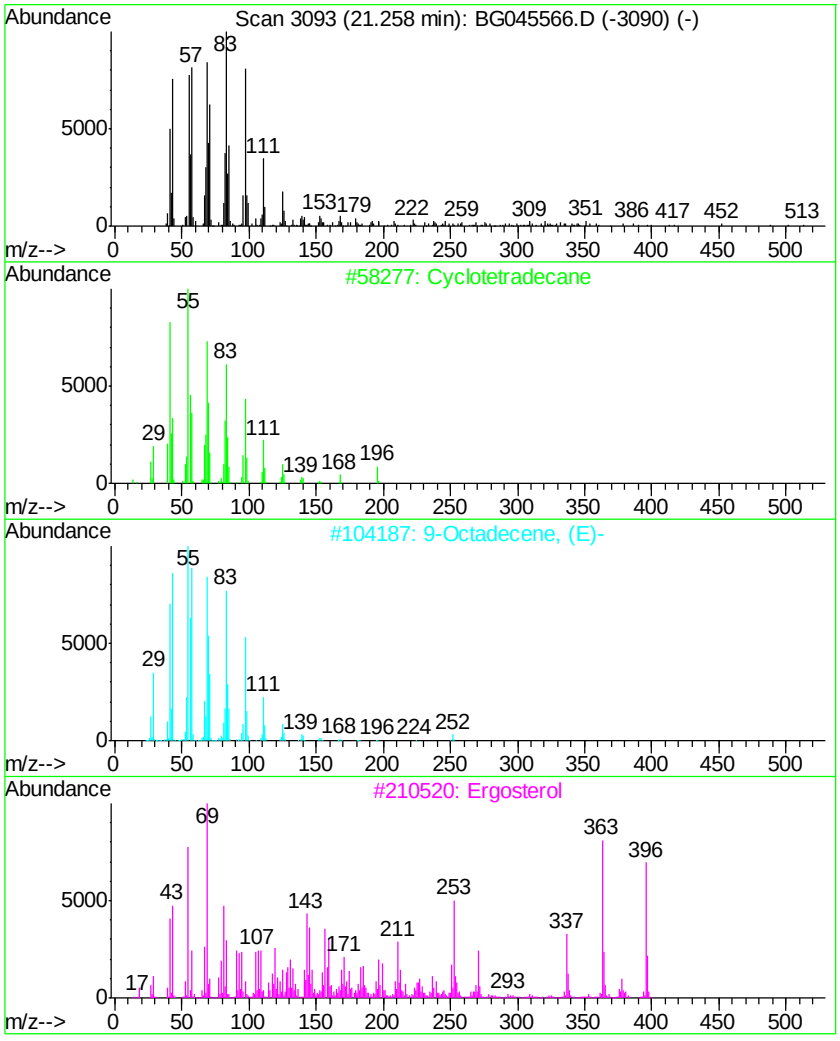
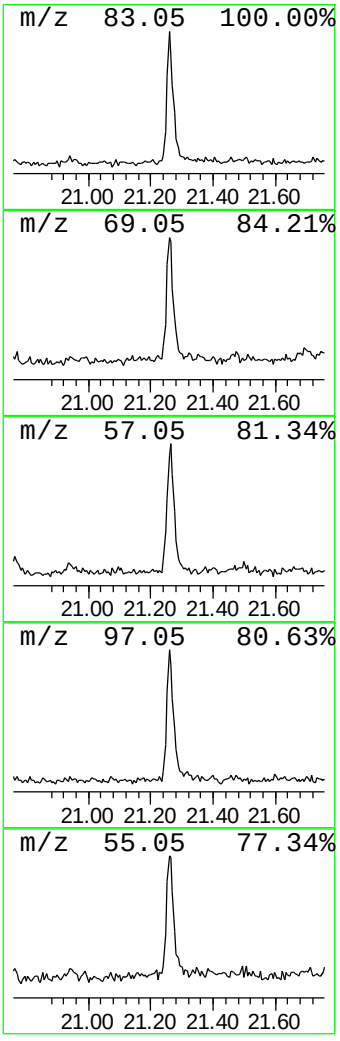
Peak Number 5 Cyclotetradecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.26	5.55 ng	372747	Chrysene-d12	21.60

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclotetradecane	196	C14H28	000295-17-0	91
2	9-Octadecene, (E)-	252	C18H36	007206-25-9	91
3	Ergosterol	396	C28H44O	000057-87-4	90
4	1-Heptadecene	238	C17H34	006765-39-5	89
5	n-Nonadecanol-1	284	C19H40O	001454-84-8	87





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG060120\
Data File : BG045566.D
Acq On : 1 Jun 2020 21:57
Operator : CG/JU
Sample : L2792-08
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : NM114-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

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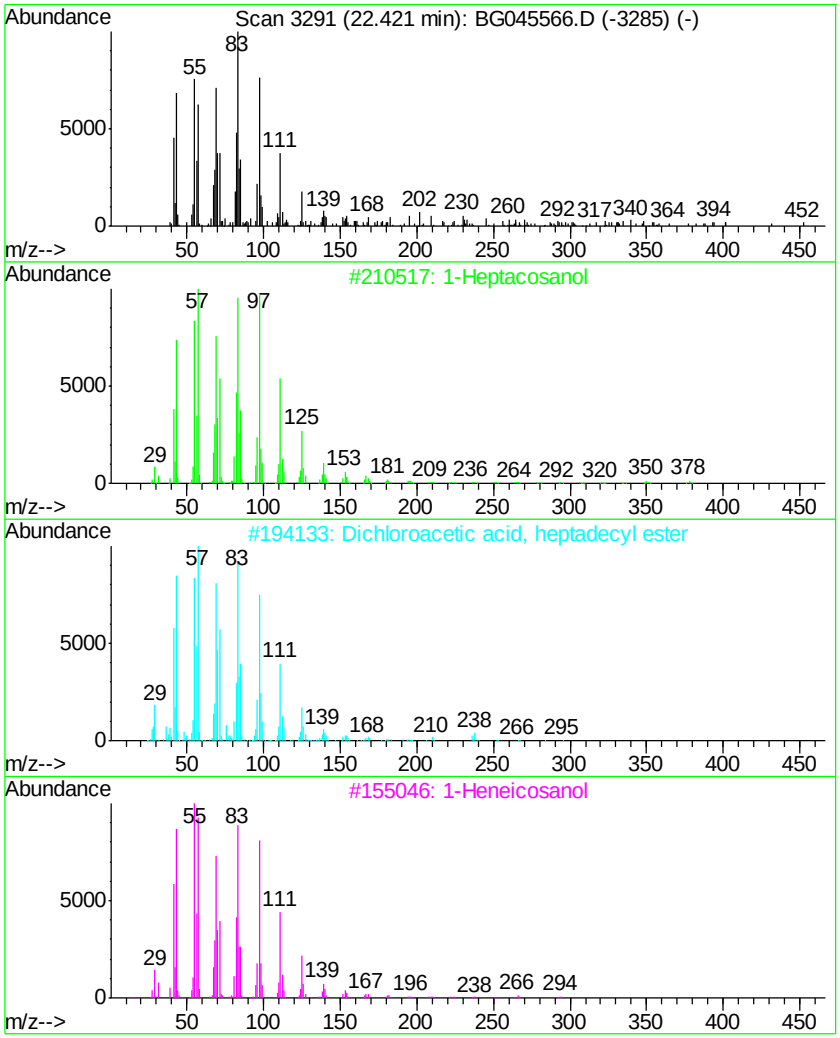
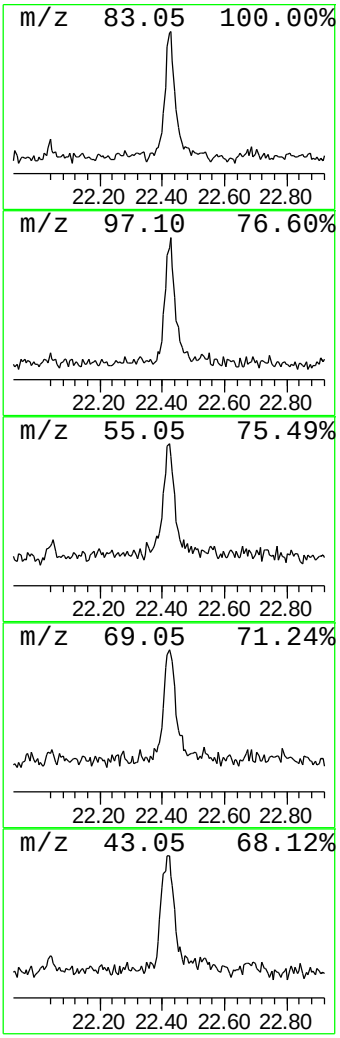
Peak Number 6 1-Heptacosanol Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.42	4.68 ng	314283	Chrysene-d12	21.60

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heptacosanol	396	C27H56O	002004-39-9	93
2	Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	91
3	1-Heneicosanol	312	C21H44O	015594-90-8	90
4	n-Tetracosanol-1	354	C24H50O	000506-51-4	90
5	1-Hexacosanol	382	C26H54O	000506-52-5	90





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Data File : BG045566.D
Acq On : 1 Jun 2020 21:57
Operator : CG/JU
Sample : L2792-08
Misc :
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Instrument : BNA_G
ClientSampleId : NM114-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

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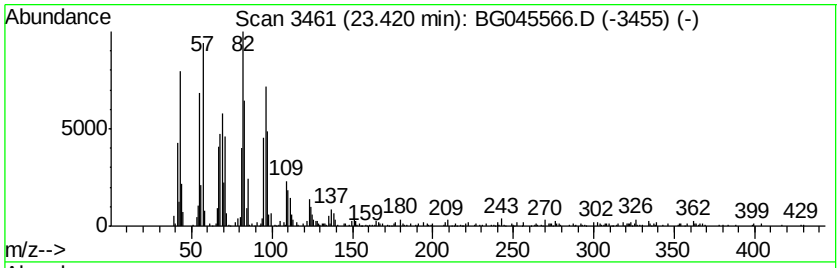
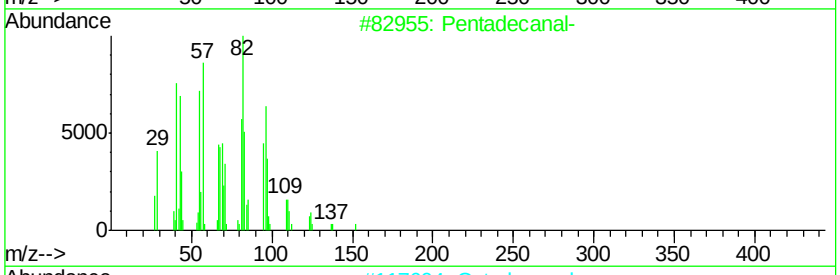
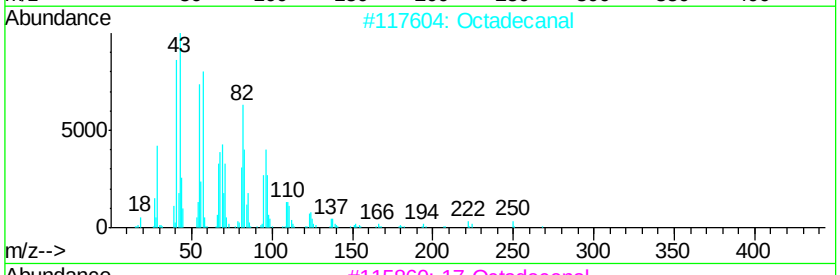
Peak Number 7 Pentadecanal- Concentration Rank 5

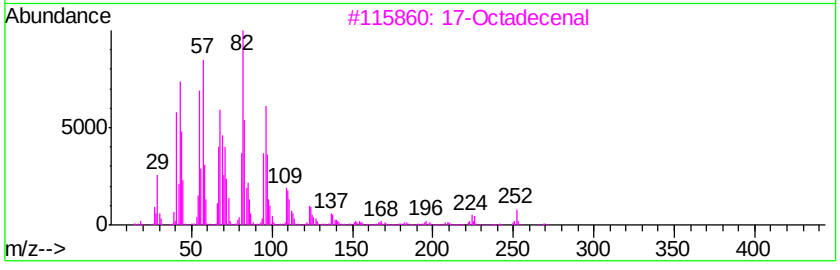
R.T.	EstConc	Area	Relative to ISTD	R.T.
23.42	9.16 ng	512383	Perylene-d12	24.75

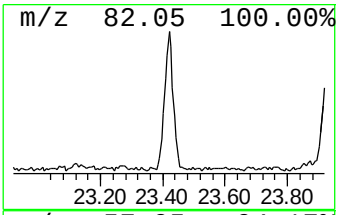
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecanal-	226	C15H30O	002765-11-9	91
2	Octadecanal	268	C18H36O	000638-66-4	91
3	17-Octadecenal	266	C18H34O	056554-86-0	90
4	Tetradecanal	212	C14H28O	000124-25-4	90
5	16-Octadecenal	266	C18H34O	056554-87-1	90

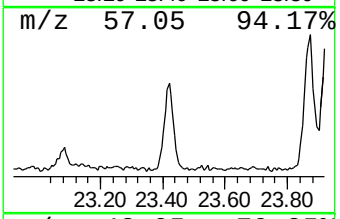


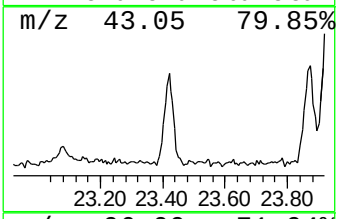


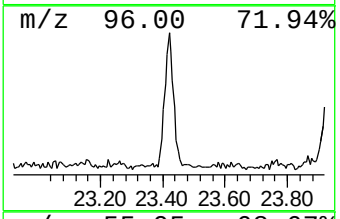


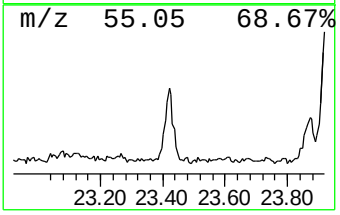












Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG060120\
Data File : BG045566.D
Acq On : 1 Jun 2020 21:57
Operator : CG/JU
Sample : L2792-08
Misc :
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Instrument : BNA_G
ClientSampleId : NM114-COMP-2020-0-6

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

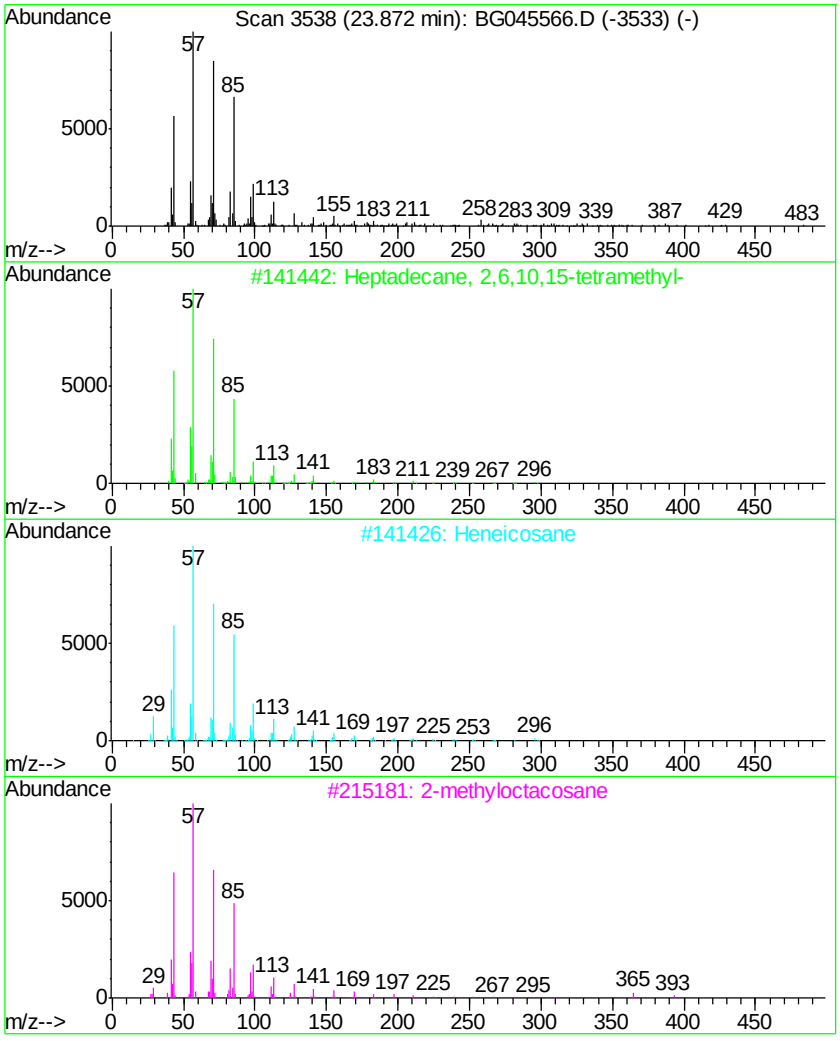
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

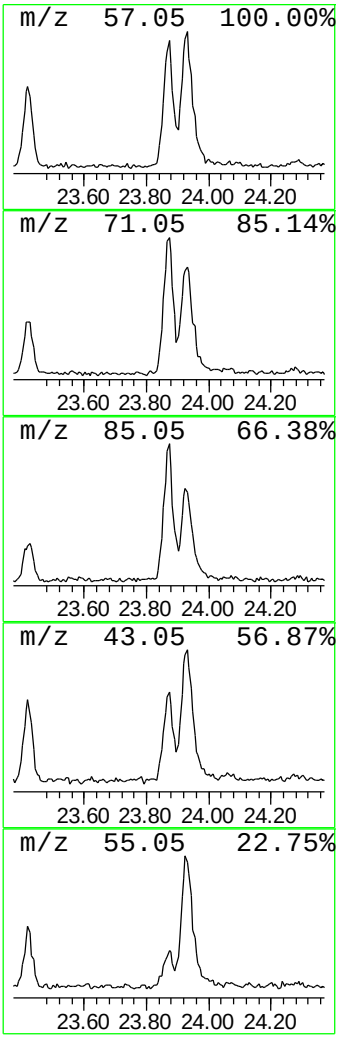
****

Peak Number 8 Heptadecane, 2,6,10,15-tetr... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.87	4.19 ng	234522	Perylene-d12	24.75

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	91
2	Heneicosane	296	C21H44	000629-94-7	91
3	2-methyloctacosane	408	C29H60	1000376-72-8	91
4	Eicosane, 10-methyl-	296	C21H44	054833-23-7	90
5	Octadecane, 1-iodo-	380	C18H37I	000629-93-6	86





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG060120\
Data File : BG045566.D
Acq On : 1 Jun 2020 21:57
Operator : CG/JU
Sample : L2792-08
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : NM114-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

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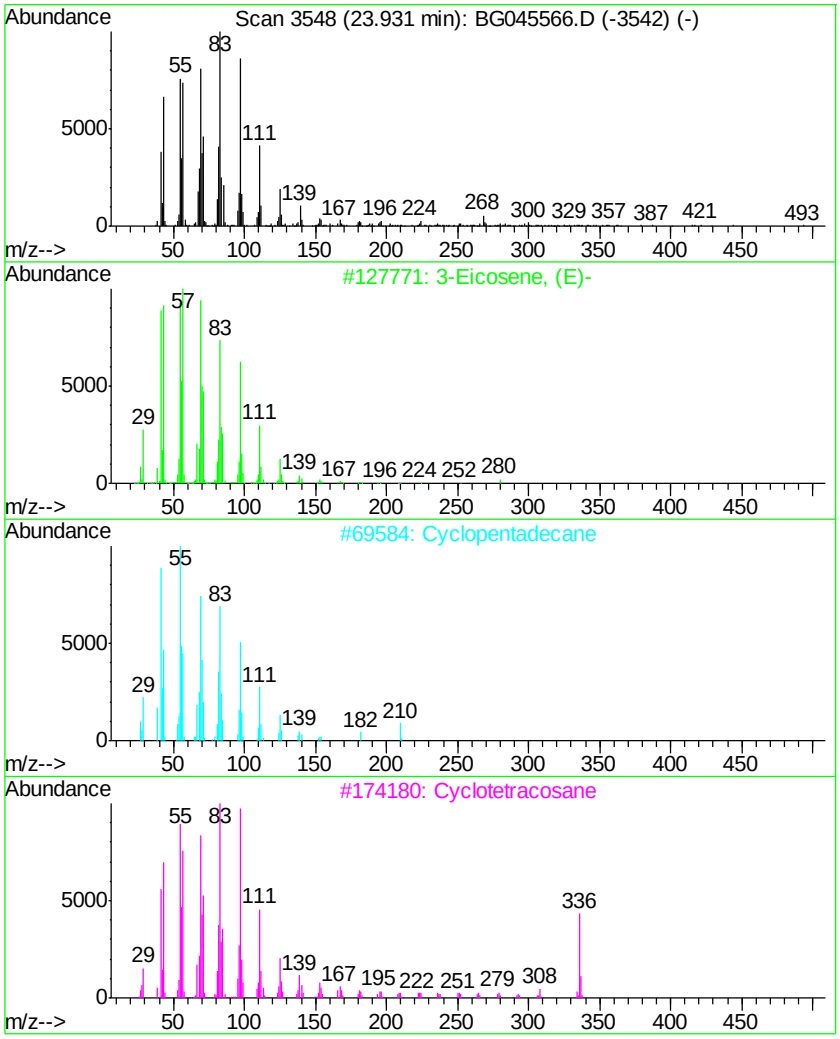
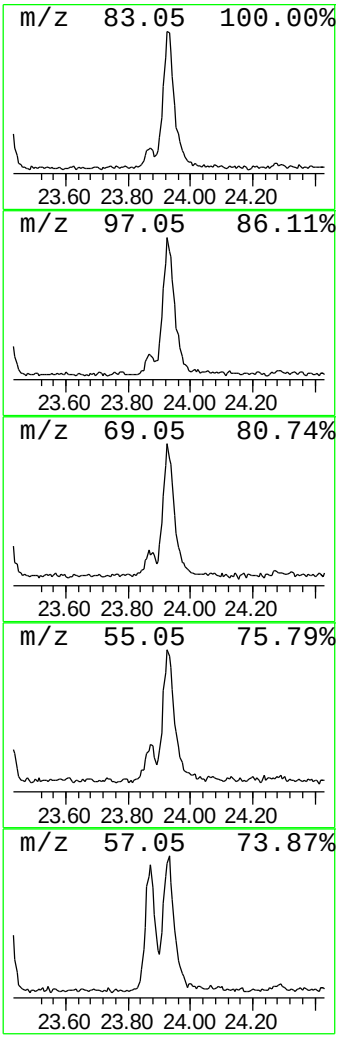
Peak Number 9 3-Eicosene, (E)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.93	16.66 ng	931810	Perylene-d12	24.75

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Eicosene, (E)-	280	C20H40	074685-33-9	93
2	Cyclopentadecane	210	C15H30	000295-48-7	93
3	Cyclotetracosane	336	C24H48	000297-03-0	83
4	Behenic alcohol	326	C22H46O	000661-19-8	81
5	1-Heneicosanol	312	C21H44O	015594-90-8	76





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Acq On : 1 Jun 2020 21:57
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Sample : L2792-08
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : NM114-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

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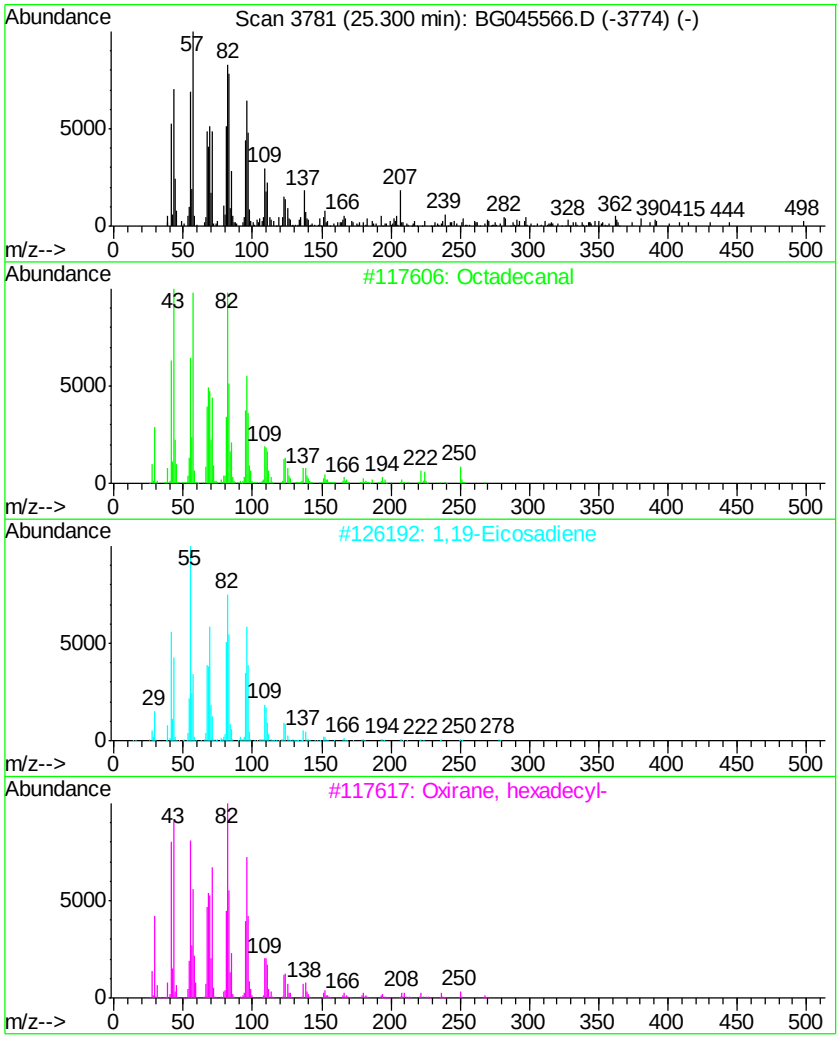
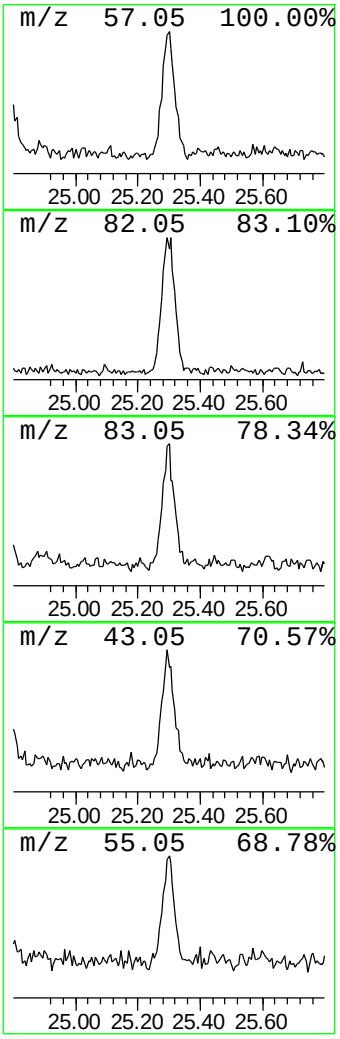
Peak Number 10 Octadecanal Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
25.30	7.03 ng	392929	Perylene-d12	24.75

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanal	268	C18H36O	000638-66-4	86
2	1,19-Eicosadiene	278	C20H38	014811-95-1	86
3	Oxirane, hexadecyl-	268	C18H36O	007390-81-0	78
4	E-11(13-Methyl)tetradecen-1-ol a...	268	C17H32O2	1000130-80-4	78
5	2-Heptadecenal	252	C17H32O	1000143-48-6	78





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG060120\
Data File : BG045566.D
Acq On : 1 Jun 2020 21:57
Operator : CG/JU
Sample : L2792-08
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : NM114-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

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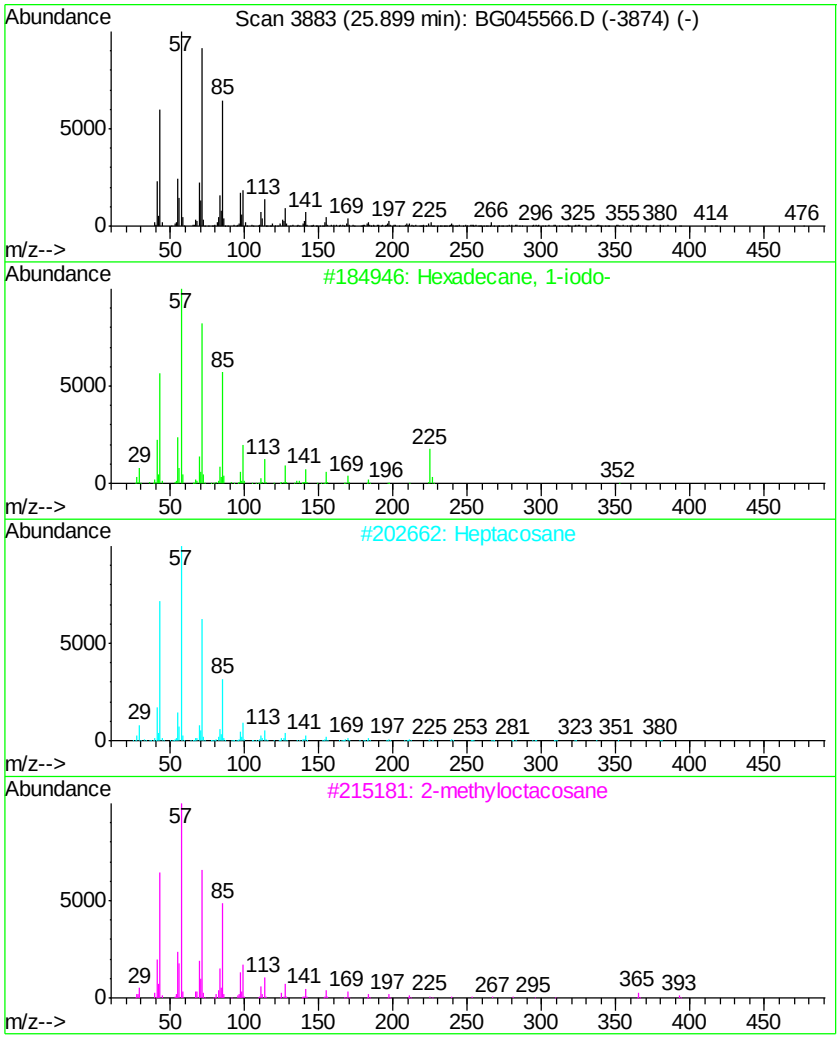
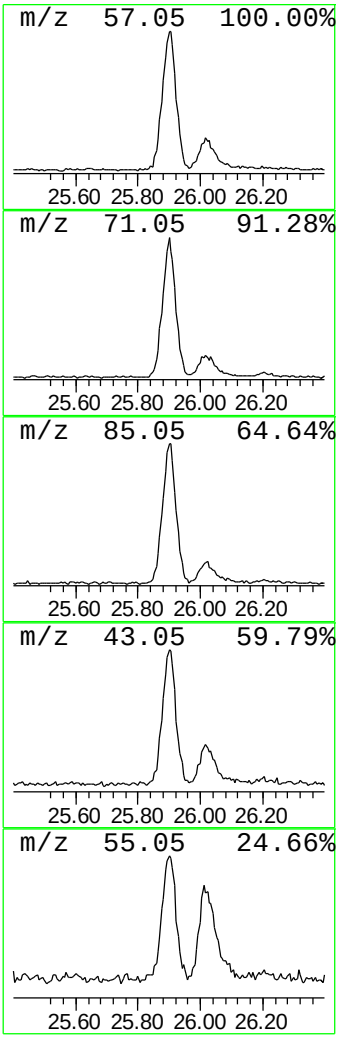
Peak Number 11 Hexadecane, 1-iodo- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
25.90	21.73 ng	1215420	Perylene-d12	24.75

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane, 1-iodo-	352	C16H33I	000544-77-4	96
2	Heptacosane	380	C27H56	000593-49-7	94
3	2-methyloctacosane	408	C29H60	1000376-72-8	91
4	Tetracosane	338	C24H50	000646-31-1	91
5	Hexacosane	366	C26H54	000630-01-3	91





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG060120\
Data File : BG045566.D
Acq On : 1 Jun 2020 21:57
Operator : CG/JU
Sample : L2792-08
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : NM114-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

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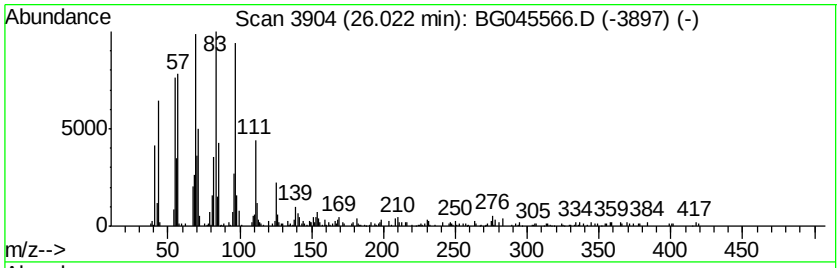
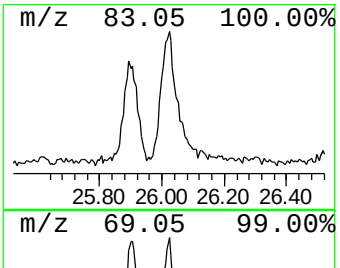
Peak Number 12 Cyclotetracosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
26.02	9.21 ng	514822	Perylene-d12	24.75

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclotetracosane	336	C24H48	000297-03-0	96
2	1-Hexacosene	364	C26H52	018835-33-1	93
3	17-Pentatriacontene	491	C35H70	006971-40-0	91
4	1-Tricosene	322	C23H46	018835-32-0	90
5	1-Heptacosanol	396	C27H56O	002004-39-9	90





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG060120\
Data File : BG045566.D
Acq On : 1 Jun 2020 21:57
Operator : CG/JU
Sample : L2792-08
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : NM114-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
1H-Cycloprop[e]az...	14.44	2.5	ng	127686	3	14.60	1026770	20.0
unknown18.25	18.25	2.3	ng	126485	4	17.35	1100180	20.0
unknown19.34	19.34	8.9	ng	489315	4	17.35	1100180	20.0
Cyclotetradecane	21.26	5.5	ng	372747	5	21.60	1342060	20.0
1-Heptacosanol	22.42	4.7	ng	314283	5	21.60	1342060	20.0
Pentadecanal-	23.42	9.2	ng	512383	6	24.75	1118430	20.0
Heptadecane, 2,6,...	23.87	4.2	ng	234522	6	24.75	1118430	20.0
3-Eicosene, (E)-	23.93	16.7	ng	931810	6	24.75	1118430	20.0
Octadecanal	25.30	7.0	ng	392929	6	24.75	1118430	20.0
Hexadecane, 1-iodo-	25.90	21.7	ng	1215420	6	24.75	1118430	20.0
Cyclotetracosane	26.02	9.2	ng	514822	6	24.75	1118430	20.0