

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG102921\
 Data File : BG050792.D
 Acq On : 30 Oct 2021 00:51
 Operator : CG/JU
 Sample : M4406-03
 Misc :
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 CHRT-27334

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-BG100621.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG050792.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.781	383	390	402	rBV	527581	893810	62.39%	7.840%
2	7.391	655	664	677	rBV	543714	986715	68.88%	8.655%
3	8.243	801	809	822	rBV	142589	251229	17.54%	2.204%
4	9.418	1001	1009	1019	rBV	336198	619547	43.25%	5.435%
5	10.817	1239	1247	1259	rBV2	18816	42213	2.95%	0.370%
6	11.069	1283	1290	1298	rBV	194483	364508	25.45%	3.197%
7	13.490	1695	1702	1709	rBV	756195	1232974	86.07%	10.816%
8	13.655	1724	1730	1737	rBV8	13119	31248	2.18%	0.274%
9	14.072	1794	1801	1803	rBV7	7319	16161	1.13%	0.142%
10	14.289	1834	1838	1840	rBV2	33050	48687	3.40%	0.427%
11	14.319	1840	1843	1847	rVB2	27166	40758	2.85%	0.358%
12	14.606	1887	1892	1896	rBV4	26387	47552	3.32%	0.417%
13	14.695	1902	1907	1912	rVB	45037	64228	4.48%	0.563%
14	14.871	1924	1937	1944	rBV	310220	560826	39.15%	4.920%
15	14.941	1945	1949	1955	rBV8	11859	28036	1.96%	0.246%
16	15.147	1980	1984	1986	rBV	16733	27185	1.90%	0.238%
17	15.353	2015	2019	2025	rBV4	32456	73895	5.16%	0.648%
18	15.652	2065	2070	2078	rVB5	56212	90393	6.31%	0.793%
19	16.087	2138	2144	2150	rBV	142693	253126	17.67%	2.220%
20	16.357	2184	2190	2198	rBV	537557	876512	61.19%	7.689%
21	16.563	2220	2225	2230	rBV	456379	682747	47.66%	5.989%
22	17.391	2361	2366	2370	rBV	580648	829685	57.92%	7.278%
23	17.621	2400	2405	2410	rVB	317660	492294	34.37%	4.318%
24	17.997	2466	2469	2474	rVB	163536	208288	14.54%	1.827%
25	20.206	2840	2845	2851	rVB	1082142	1432529	100.00%	12.566%
26	21.921	3132	3137	3143	rVB2	284926	471514	32.91%	4.136%
27	23.666	3430	3434	3442	rVB	112371	214982	15.01%	1.886%
28	25.347	3713	3720	3731	rVB2	171564	518319	36.18%	4.547%

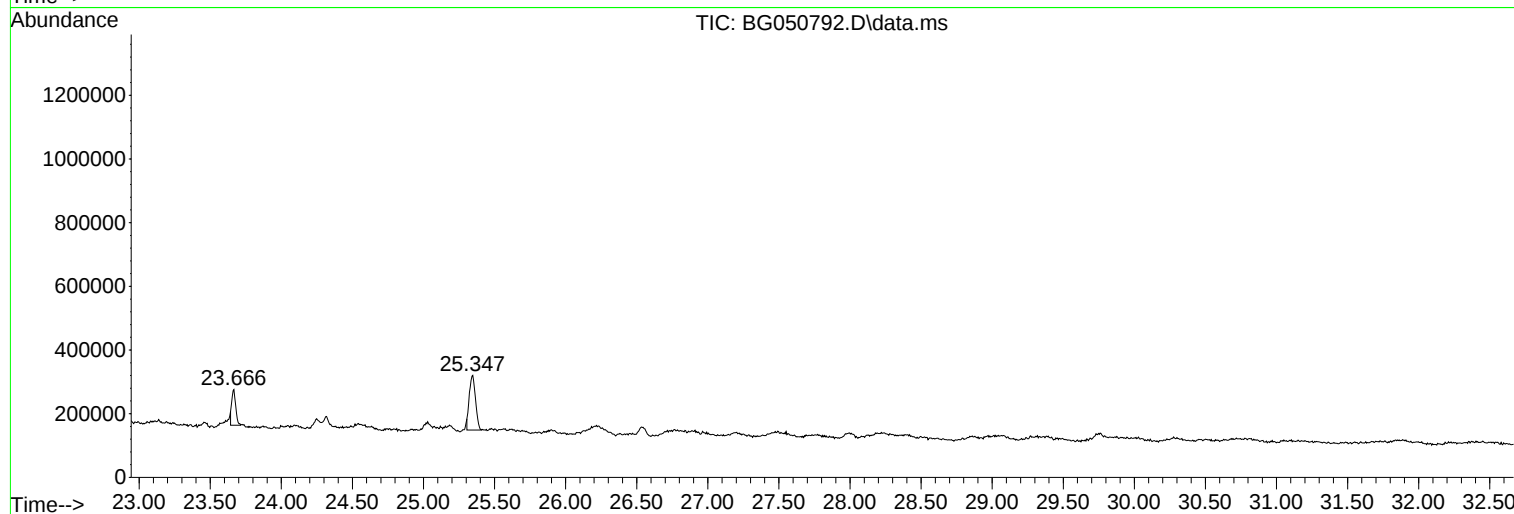
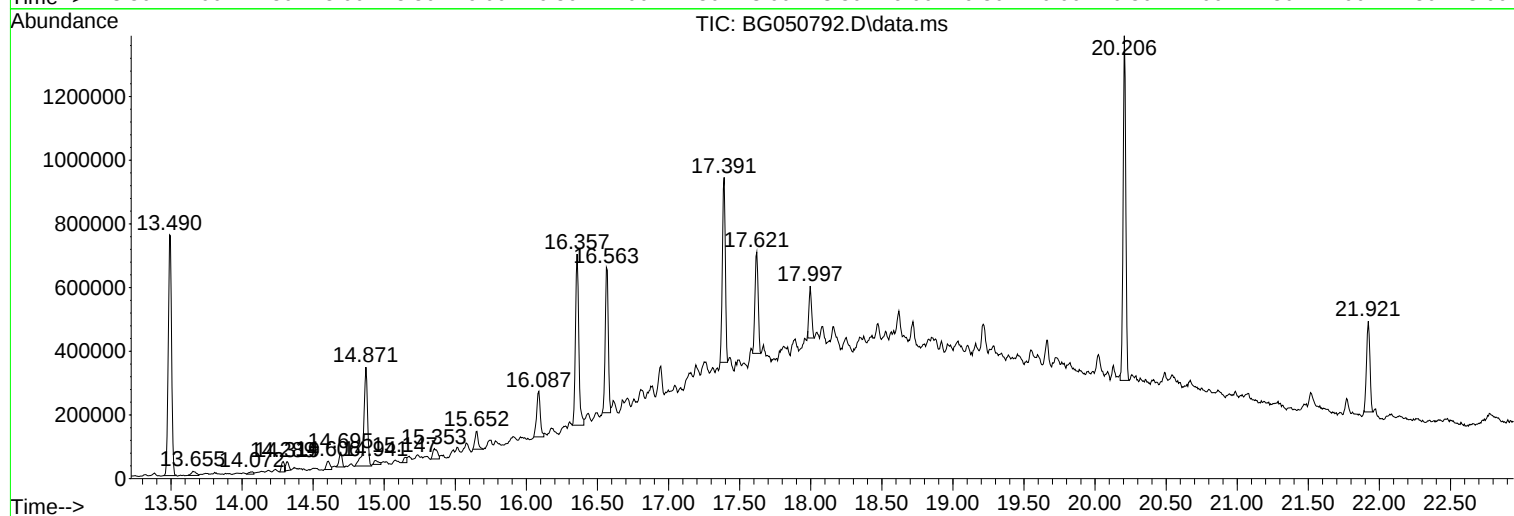
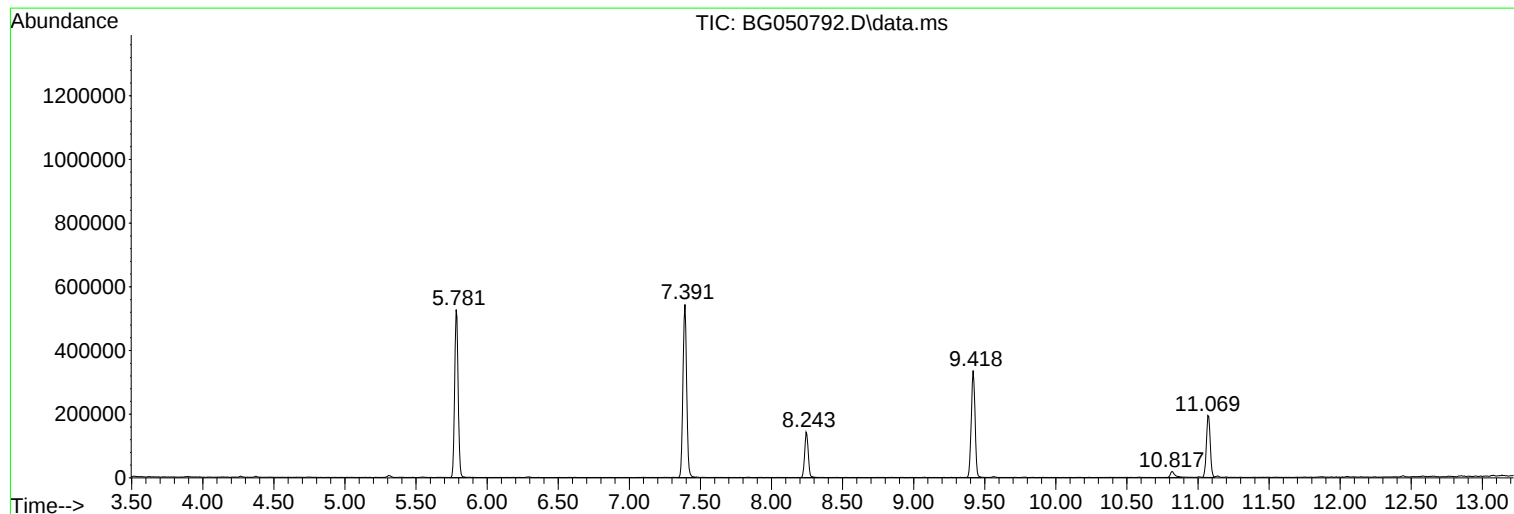
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Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
CHRT-27334

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG100621.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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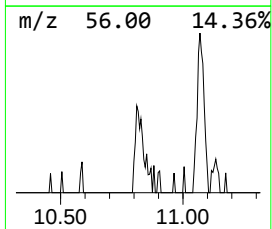
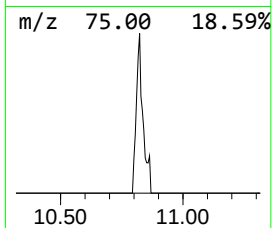
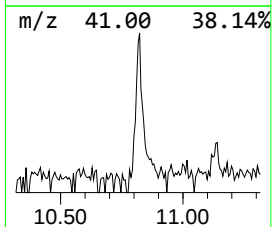
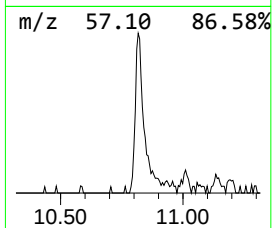
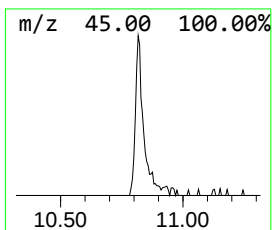
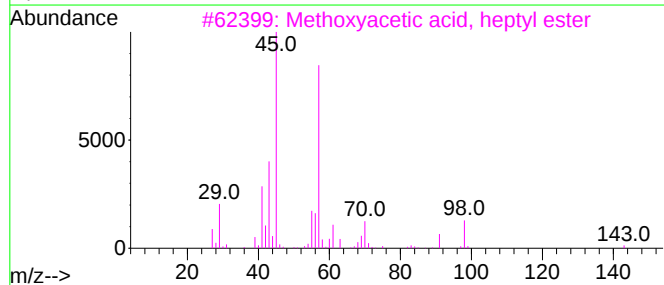
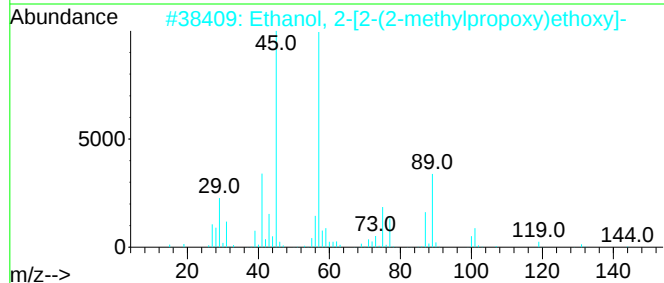
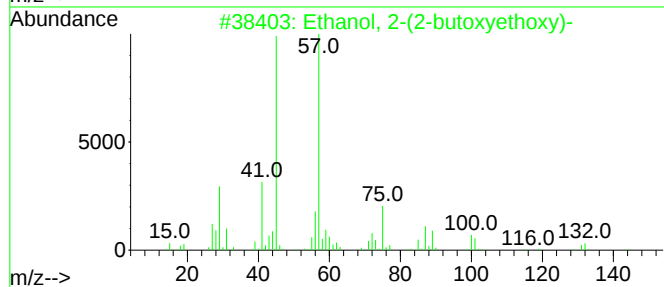
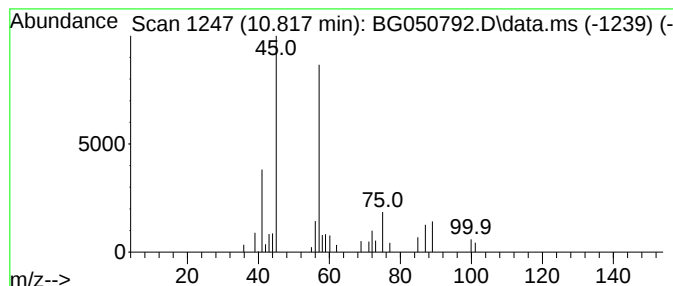
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG100621.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.817	2.32 ng	42213	Naphthalene-d8	11.069

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
2			Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	50
3			Methoxyacetic acid, heptyl ester	188	C10H20O3	168920-36-3	47
4			Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	45
5			Ethylene glycol diglycidyl ether	174	C8H14O4	002224-15-9	38



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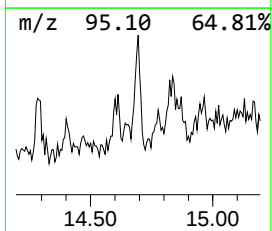
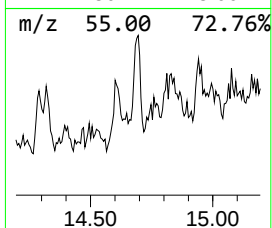
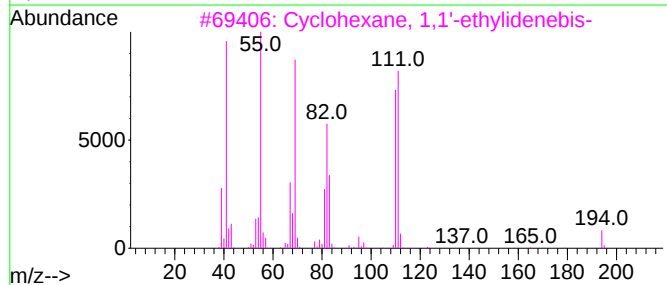
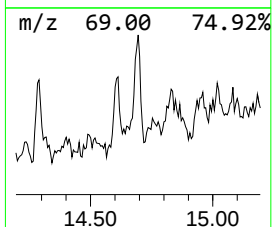
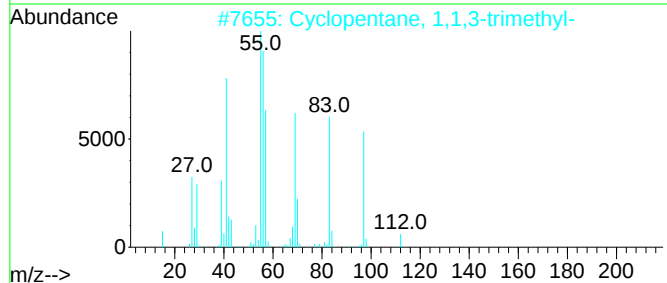
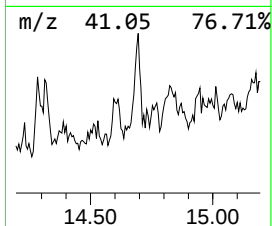
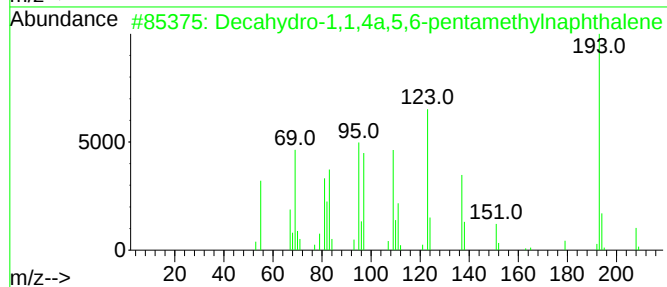
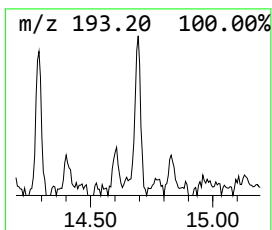
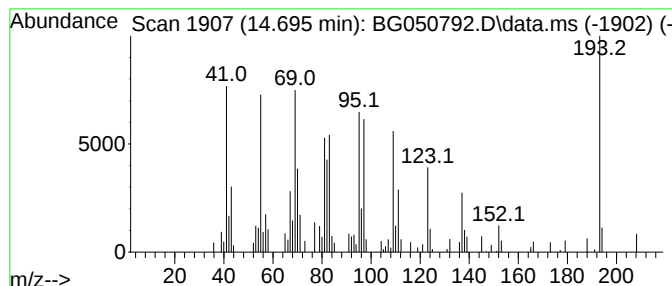
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Peak Number 2 unknown14.695 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.695	2.29 ng	64228	Acenaphthene-d10	14.871

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Decahydro-1,1,4a,5,6-pentamethyl...	208	C15H28	080655-44-3	38
2			Cyclopentane, 1,1,3-trimethyl-	112	C8H16	004516-69-2	35
3			Cyclohexane, 1,1'-ethylidenebis-	194	C14H26	002319-61-1	25
4			Cyclohexane, 1-(cyclohexylmethyl...	208	C15H28	054934-92-8	25
5			Bicyclo[3.1.1]heptan-3-one, 2,6,...	152	C10H16O	000547-60-4	18



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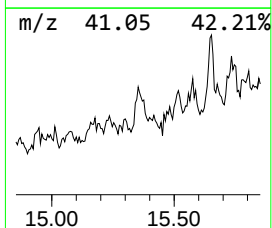
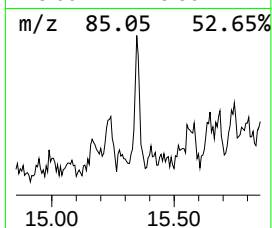
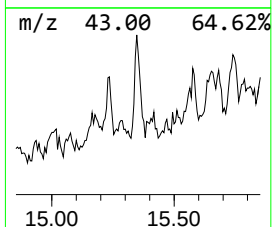
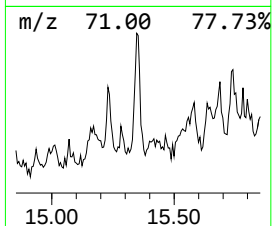
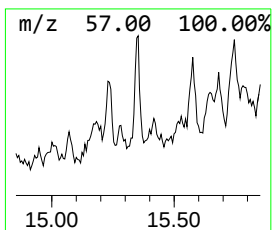
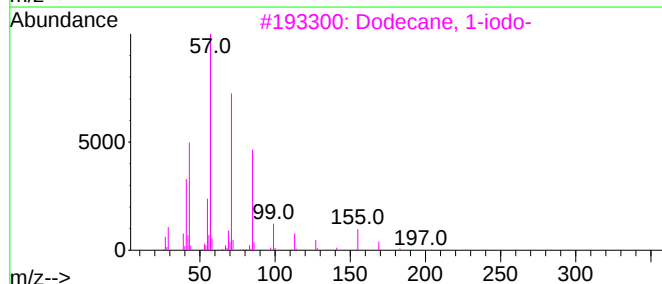
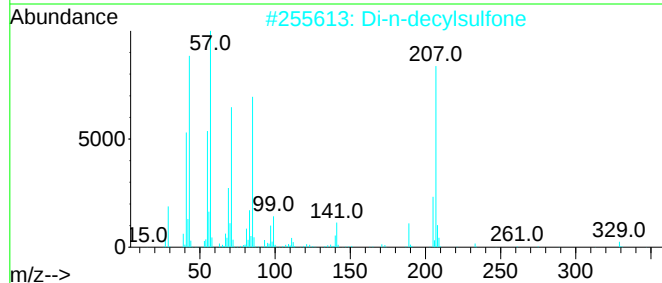
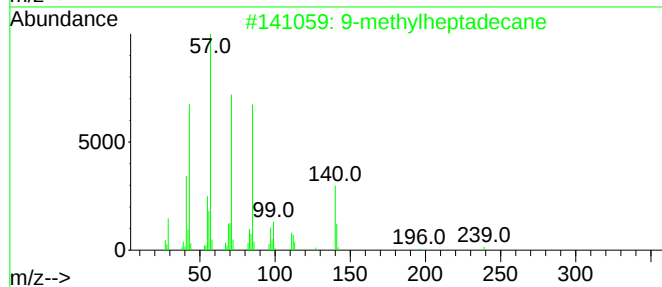
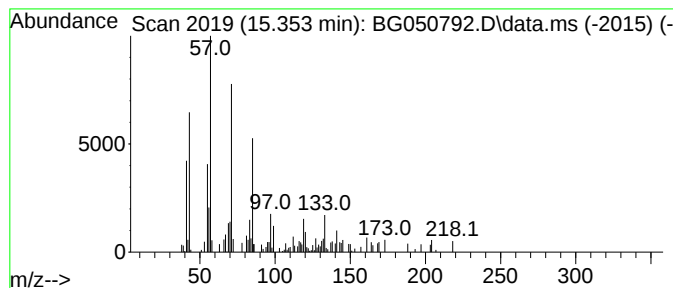
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 9-methylheptadecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.353	2.64 ng	73895	Acenaphthene-d10	14.871

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			9-methylheptadecane	254	C18H38	026741-18-4	74
2			Di-n-decylsulfone	346	C20H42O2S	111530-37-1	72
3			Dodecane, 1-iodo-	296	C12H25I	004292-19-7	64
4			Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	64
5			Decane, 1-iodo-	268	C10H21I	002050-77-3	59



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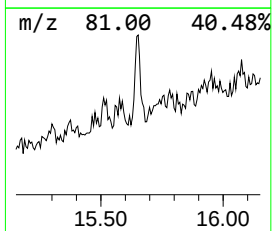
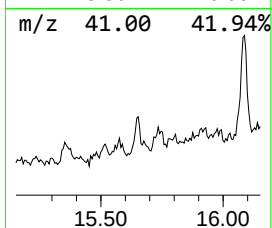
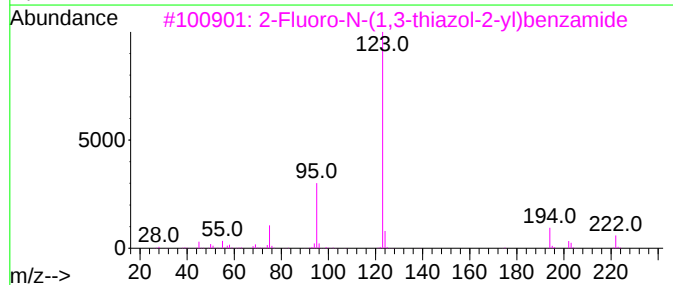
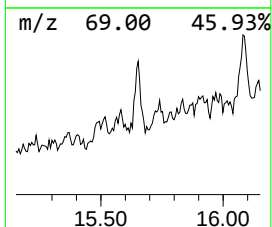
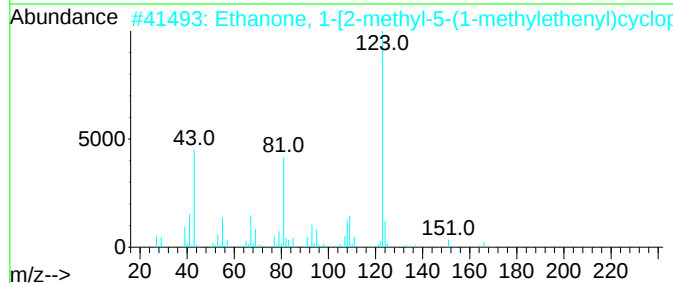
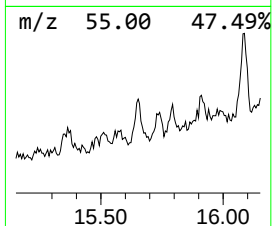
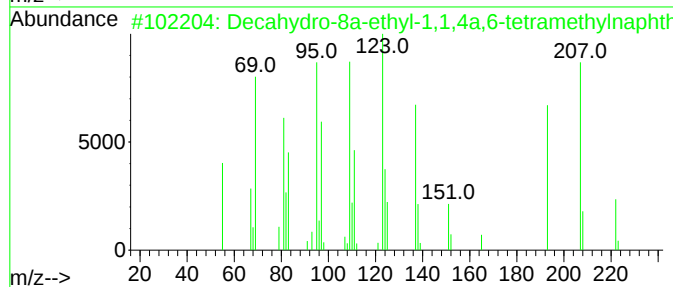
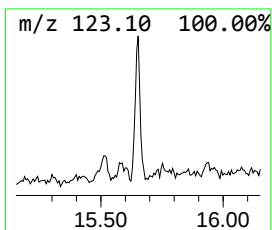
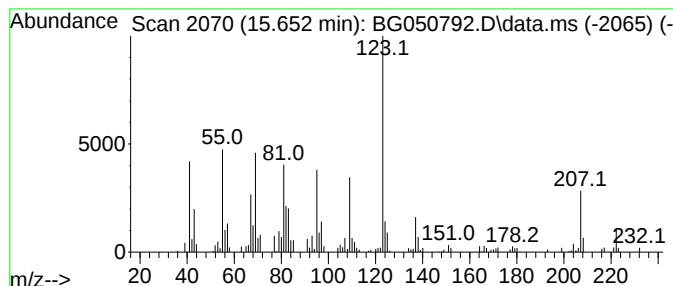
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Peak Number 4 Decahydro-8a-ethyl-1,1,4a,6... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.652	3.22 ng	90393	Acenaphthene-d10	14.871

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Decahydro-8a-ethyl-1,1,4a,6-tetr...	222	C16H30	1000100-23-6	58
2			Ethanone, 1-[2-methyl-5-(1-methy...	166	C11H18O	074063-72-2	49
3			2-Fluoro-N-(1,3-thiazol-2-yl)ben...	222	C10H7FN2OS	000319-38-0	47
4			1-(4-Fluorobenzoyl)piperazine	208	C11H13FN2O	102391-98-0	46
5			2-Pyrimidinamine, 4,6-dimethyl-	123	C6H9N3	000767-15-7	46



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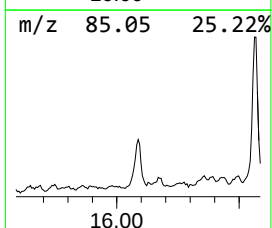
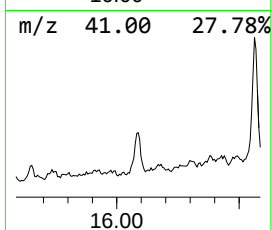
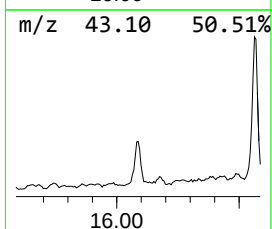
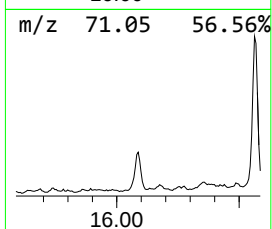
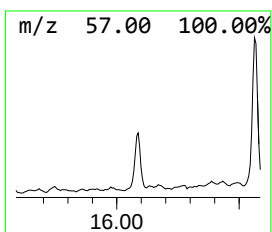
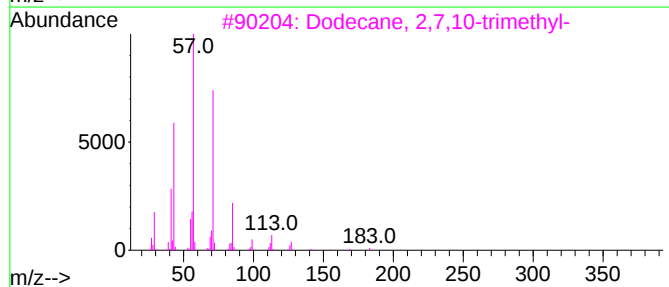
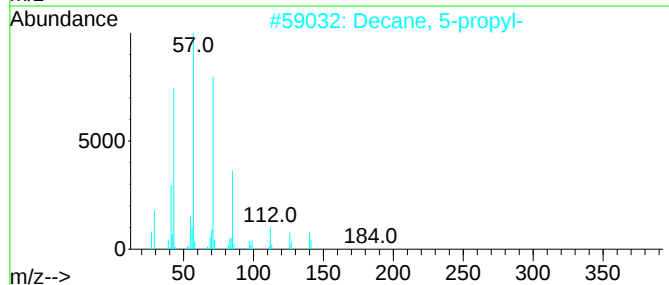
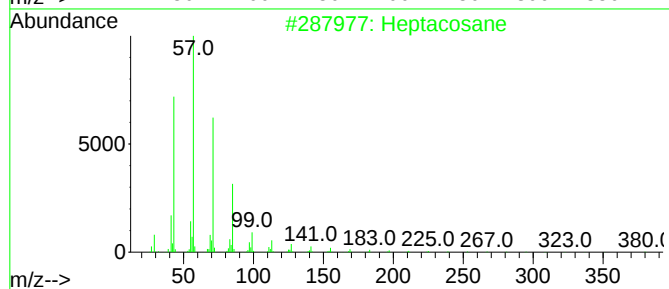
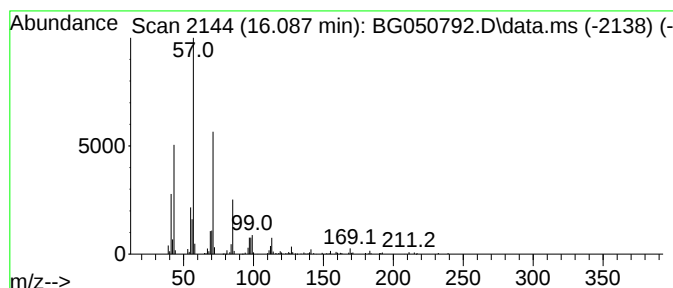
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Peak Number 5 Heptacosane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.	
16.087	9.03 ng	253126	Acenaphthene-d10	14.871	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptacosane	380	C27H56	000593-49-7	86
2	Decane, 5-propyl-	184	C13H28	017312-62-8	74
3	Dodecane, 2,7,10-trimethyl-	212	C15H32	074645-98-0	72
4	Heneicosane	296	C21H44	000629-94-7	72
5	Dodecane, 4-methyl-	184	C13H28	006117-97-1	68



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ALS Vial : 17 Sample Multiplier: 1

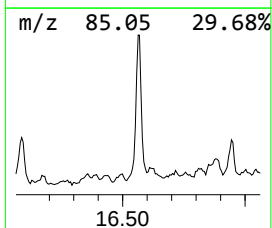
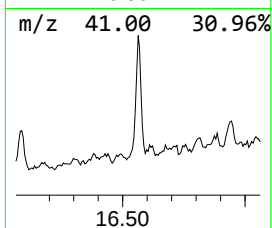
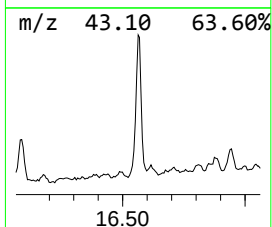
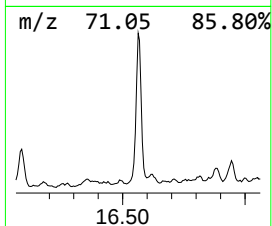
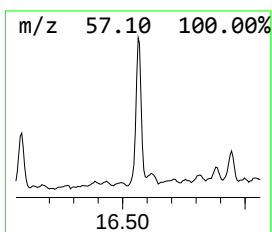
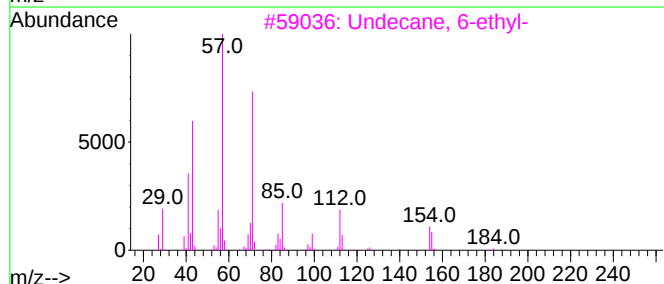
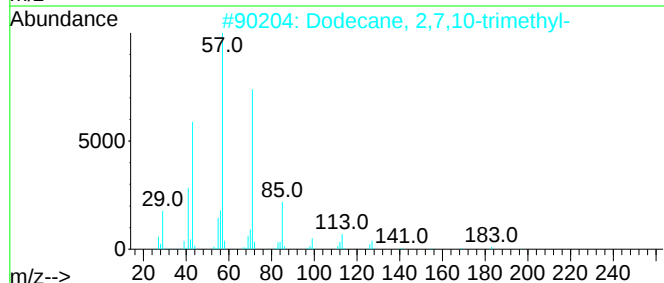
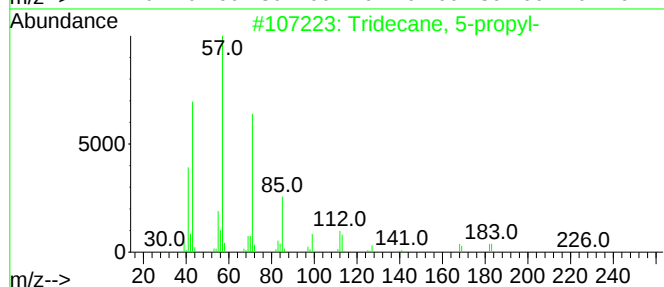
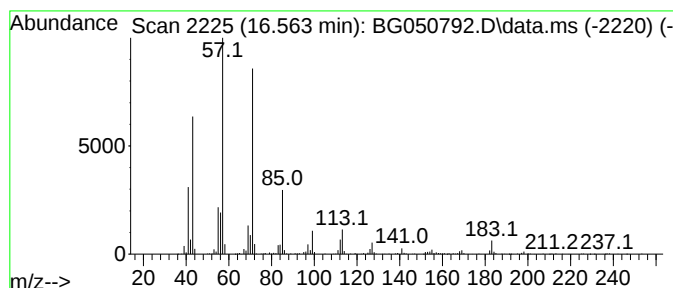
Instrument :
BNA_G
ClientSampleId :
CHRT-27334

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG100621.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Tridecane, 5-propyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
16.563	27.74 ng	682747	Phenanthrene-d10	17.621	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecane, 5-propyl-	226	C16H34	055045-11-9	93
2	Dodecane, 2,7,10-trimethyl-	212	C15H32	074645-98-0	86
3	Undecane, 6-ethyl-	184	C13H28	017312-60-6	83
4	Hexadecane, 2,6,10-trimethyl-	268	C19H40	055000-52-7	80
5	Dodecane, 2,6,11-trimethyl-	212	C15H32	031295-56-4	72



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG102921\
Data File : BG050792.D
Acq On : 30 Oct 2021 00:51
Operator : CG/JU
Sample : M4406-03
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
CHRT-27334

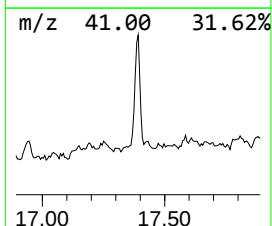
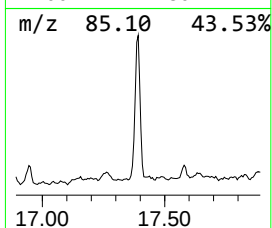
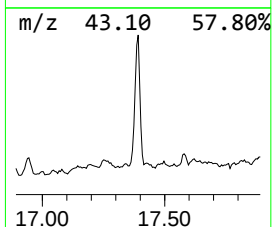
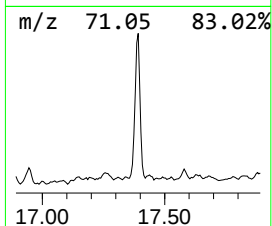
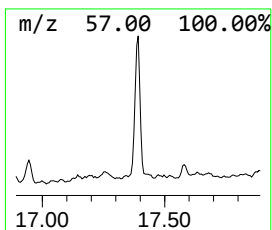
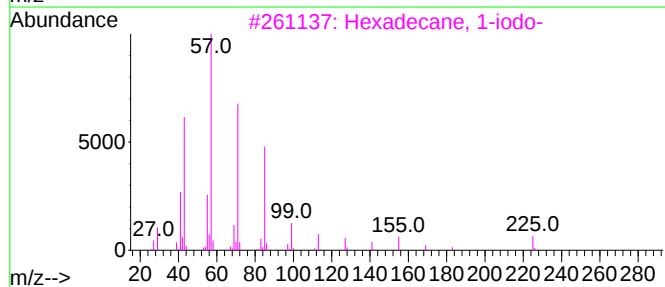
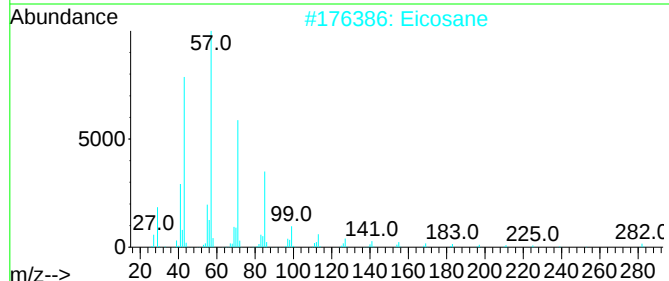
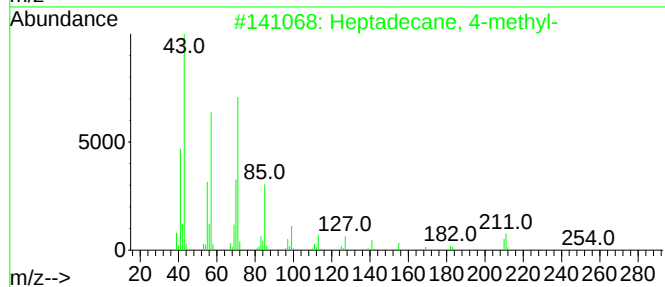
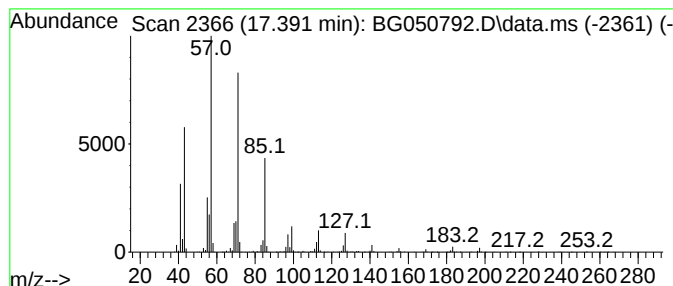
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Heptadecane, 4-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.391	33.71 ng	829685	Phenanthrene-d10	17.621

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptadecane, 4-methyl-	254	C18H38	026429-11-8	90
2			Eicosane	282	C20H42	000112-95-8	90
3			Hexadecane, 1-iodo-	352	C16H33I	000544-77-4	90
4			Octadecane, 1-iodo-	380	C18H37I	000629-93-6	90
5			Tetradecane, 1-iodo-	324	C14H29I	019218-94-1	86



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG102921\
Data File : BG050792.D
Acq On : 30 Oct 2021 00:51
Operator : CG/JU
Sample : M4406-03
Misc :
ALS Vial : 17 Sample Multiplier: 1

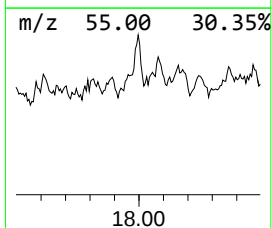
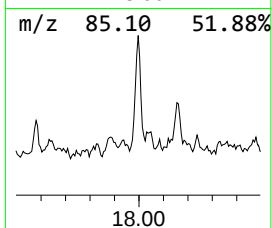
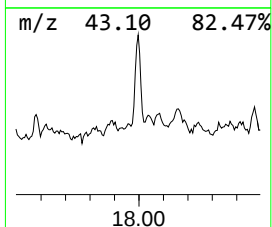
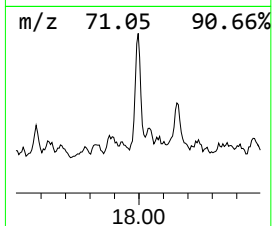
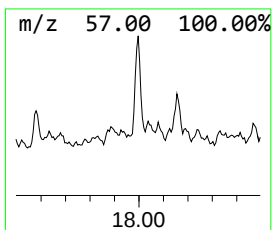
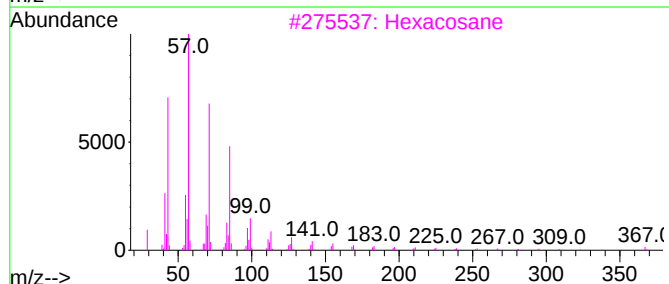
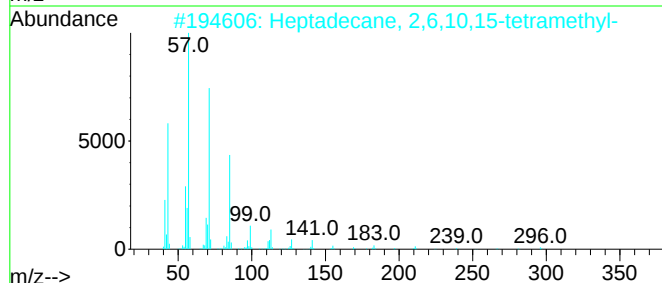
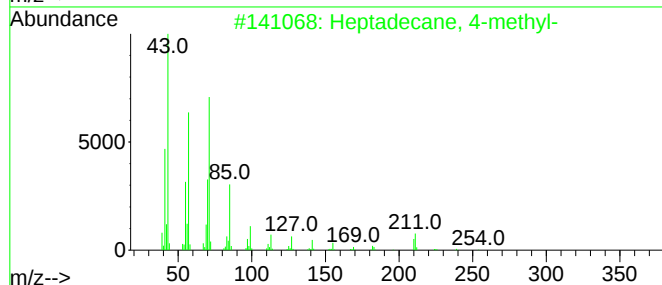
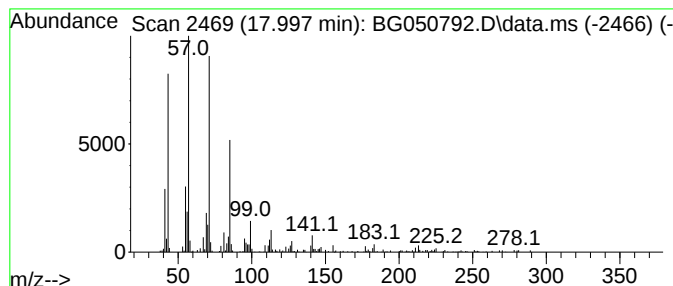
Instrument :
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ClientSampleId :
CHRT-27334

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG100621.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Heptadecane, 2,6,10,15-tetr... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
17.997	8.46 ng	208288	Phenanthrene-d10	17.621	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane, 4-methyl-	254	C18H38	026429-11-8	91
2	Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	91
3	Hexacosane	366	C26H54	000630-01-3	90
4	Nonadecane	268	C19H40	000629-92-5	87
5	Tetradecane	198	C14H30	000629-59-4	86



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG102921\
Data File : BG050792.D
Acq On : 30 Oct 2021 00:51
Operator : CG/JU
Sample : M4406-03
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
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ClientSampleId :
CHRT-27334

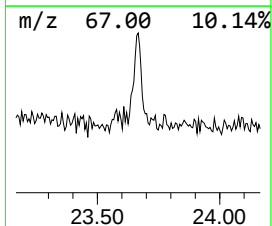
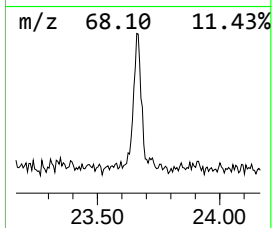
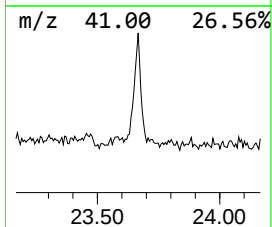
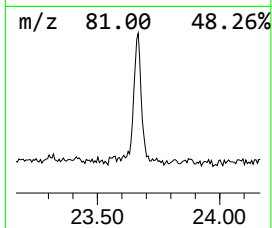
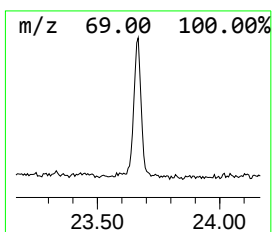
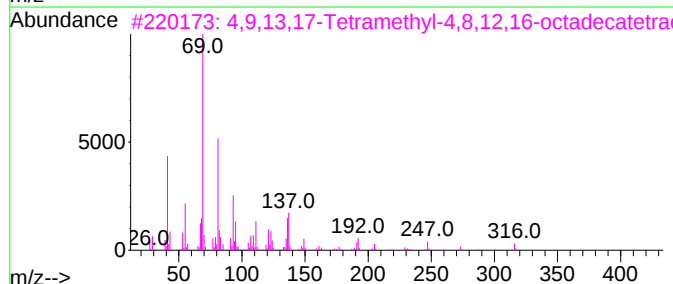
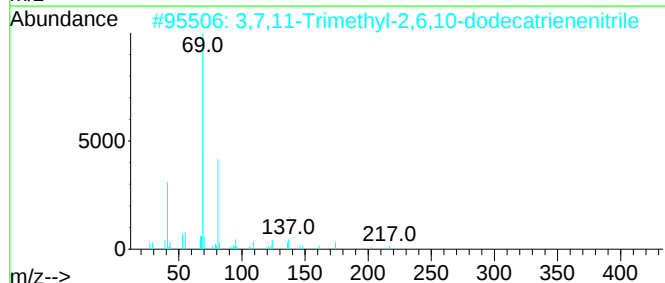
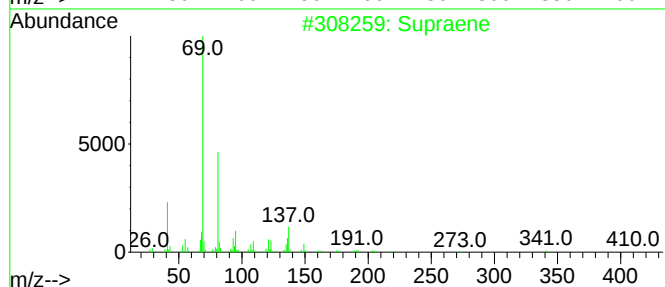
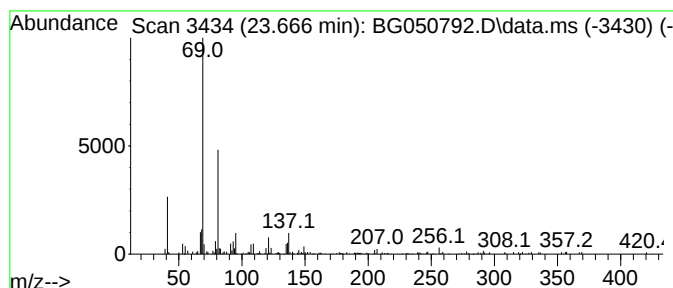
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Supraene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.666	8.30 ng	214982	Perylene-d12	25.347

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Supraene	410	C30H50	007683-64-9	86
2			3,7,11-Trimethyl-2,6,10-dodecatr...	217	C15H23N	029789-67-1	72
3			4,9,13,17-Tetramethyl-4,8,12,16-...	316	C22H36O	056882-09-8	64
4			4,8,12-Tetradecatrienal, 5,9,13-...	248	C17H28O	066408-55-7	64
5			1,5-Heptadiene, 3,3,6-trimethyl-	138	C10H18	035387-63-4	53



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG102921\
Data File : BG050792.D
Acq On : 30 Oct 2021 00:51
Operator : CG/JU
Sample : M4406-03
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
CHRT-27334

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG100621.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Ethanol, 2-(2-b...	10.817	2.3	ng	42213	2	11.069	364508	20.0
unknown14.695	14.695	2.3	ng	64228	3	14.871	560826	20.0
9-methylheptade...	15.353	2.6	ng	73895	3	14.871	560826	20.0
Decahydro-8a-et...	15.652	3.2	ng	90393	3	14.871	560826	20.0
Heptacosane	16.087	9.0	ng	253126	3	14.871	560826	20.0
Tridecane, 5-pr...	16.563	27.7	ng	682747	4	17.621	492294	20.0
Heptadecane, 4-...	17.391	33.7	ng	829685	4	17.621	492294	20.0
Heptadecane, 2,...	17.997	8.5	ng	208288	4	17.621	492294	20.0
Supraene	23.666	8.3	ng	214982	6	25.347	518319	20.0