

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG041824\
 Data File : BG060945.D
 Acq On : 18 Apr 2024 21:19
 Operator : MA/JU
 Sample : P2166-03
 Misc :
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 RPI-SS-DUP-01

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-BG041724.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG060945.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.160	24	29	37	rBV	99141	150210	3.38%	0.701%
2	3.671	111	116	126	rBV	50607	78665	1.77%	0.367%
3	5.528	424	432	442	rBV	1025970	1571142	35.33%	7.337%
4	7.109	692	701	709	rBV	1060683	1799340	40.46%	8.403%
5	7.937	835	842	848	rBV	192445	317520	7.14%	1.483%
6	9.094	1029	1039	1046	rBV	631027	1090561	24.52%	5.093%
7	10.505	1273	1279	1290	rBV2	26014	45848	1.03%	0.214%
8	10.734	1309	1318	1326	rBV	244157	425848	9.58%	1.989%
9	11.474	1437	1444	1449	rBV3	25307	47511	1.07%	0.222%
10	13.190	1729	1736	1744	rBV	1595963	2453607	55.18%	11.458%
11	14.565	1964	1970	1982	rVB	478789	708833	15.94%	3.310%
12	14.770	1996	2005	2007	rBV2	31755	48194	1.08%	0.225%
13	16.057	2216	2224	2232	rBV	1699962	2675946	60.17%	12.496%
14	17.314	2431	2438	2447	rVB	672730	1011398	22.74%	4.723%
15	18.219	2586	2592	2600	rBV	329838	483892	10.88%	2.260%
16	19.494	2804	2809	2817	rBV	131099	205793	4.63%	0.961%
17	19.935	2878	2884	2894	rBV	3342709	4446941	100.00%	20.766%
18	21.251	3102	3108	3118	rBV2	196759	373491	8.40%	1.744%
19	21.568	3156	3162	3174	rVB2	722337	1149792	25.86%	5.369%
20	21.797	3197	3201	3207	rVB	46070	63648	1.43%	0.297%
21	22.397	3299	3303	3314	rVB4	62307	142145	3.20%	0.664%
22	23.254	3444	3449	3456	rVB2	55707	108048	2.43%	0.505%
23	23.865	3547	3553	3559	rBV	78376	163983	3.69%	0.766%
24	24.688	3683	3693	3704	rBV	438480	1247184	28.05%	5.824%
25	25.898	3891	3899	3908	rBV2	97594	292411	6.58%	1.366%
26	26.004	3912	3917	3923	rBV10	19222	55152	1.24%	0.258%
27	28.836	4390	4399	4413	rVB5	59162	256972	5.78%	1.200%

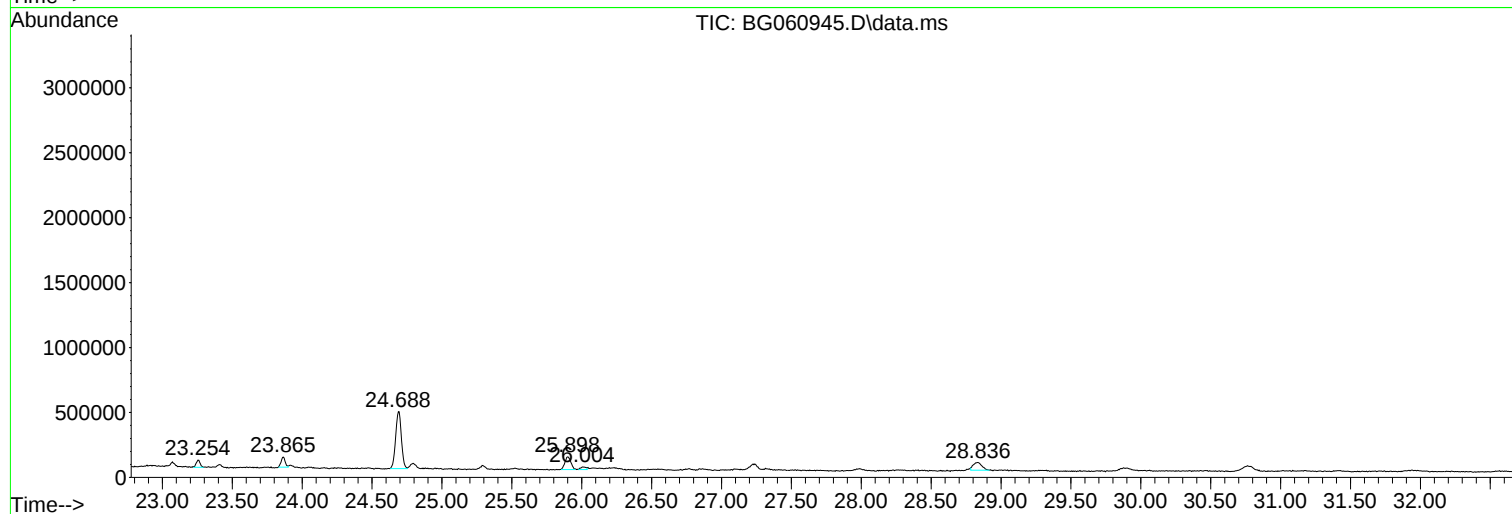
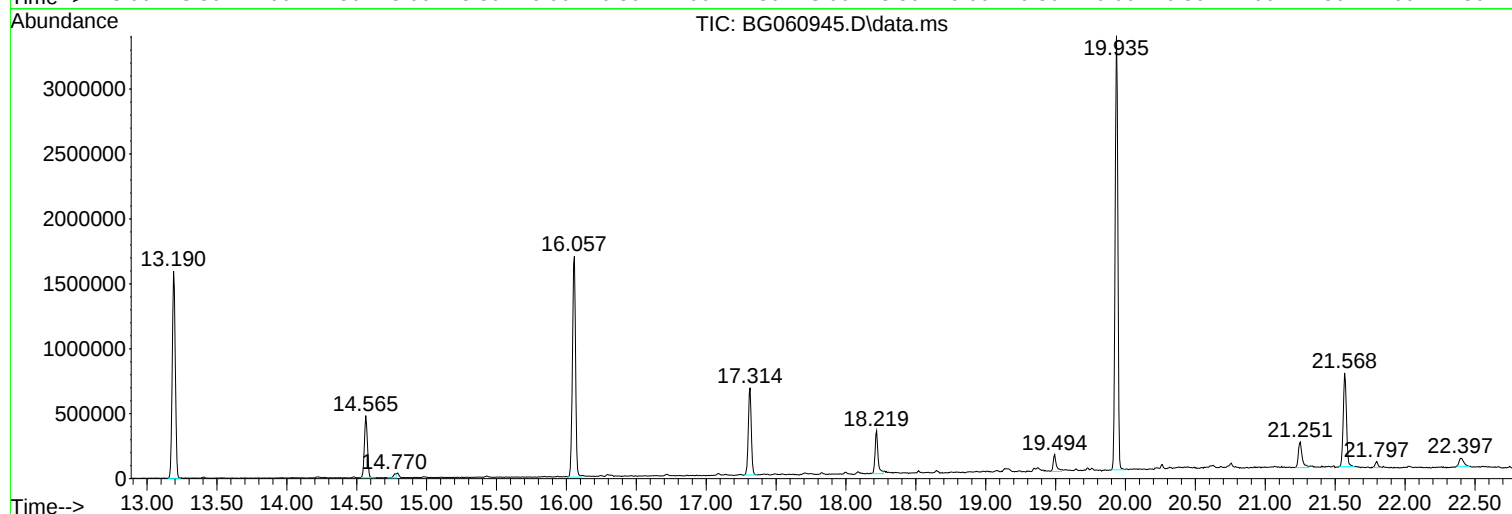
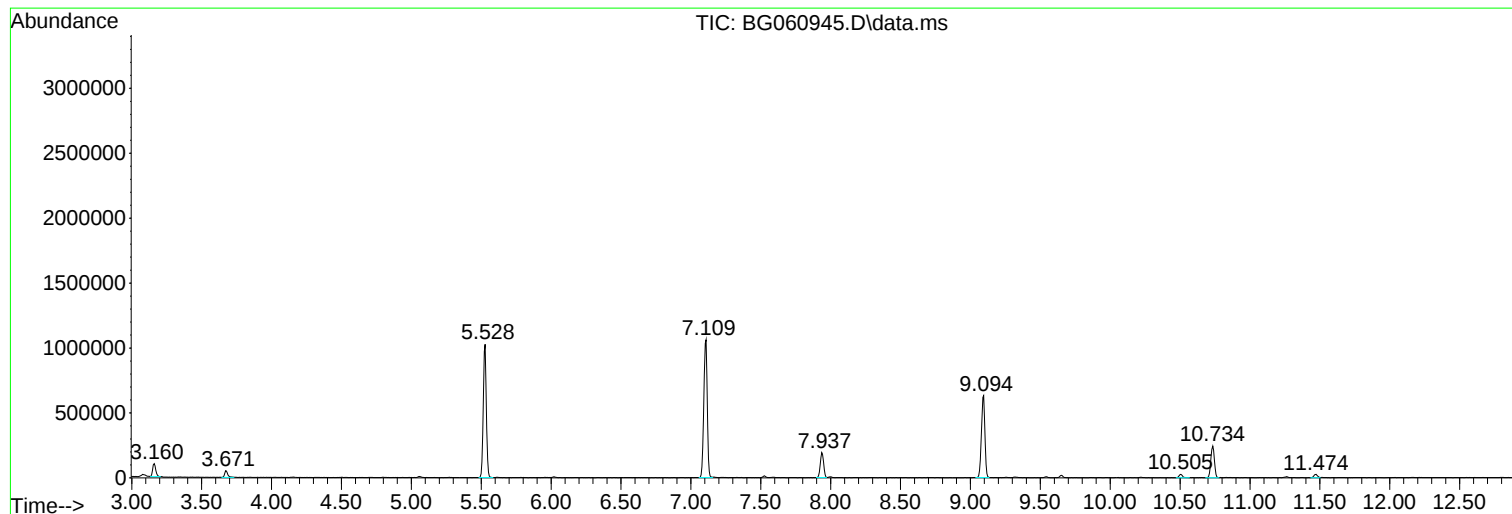
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG041724.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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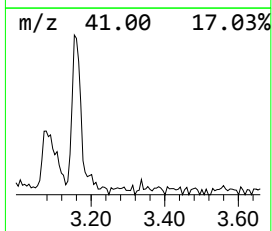
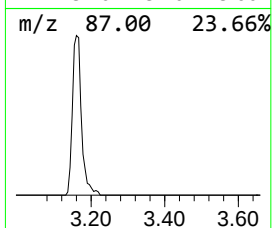
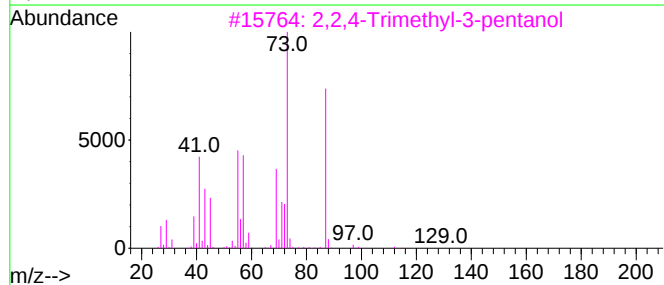
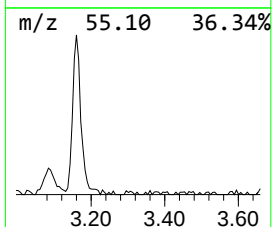
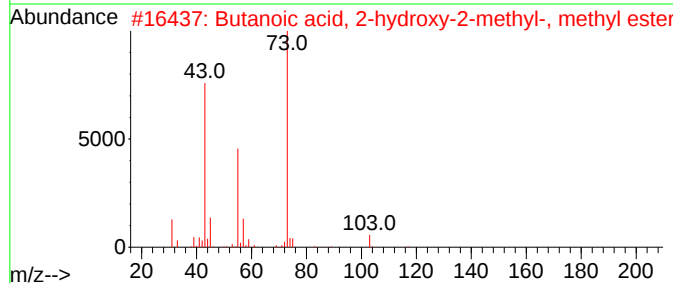
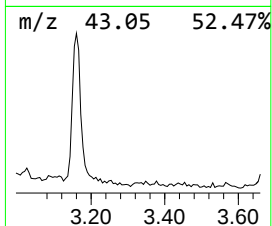
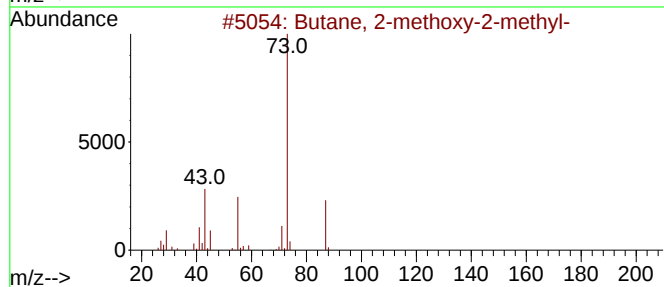
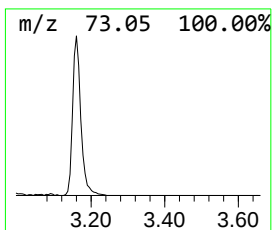
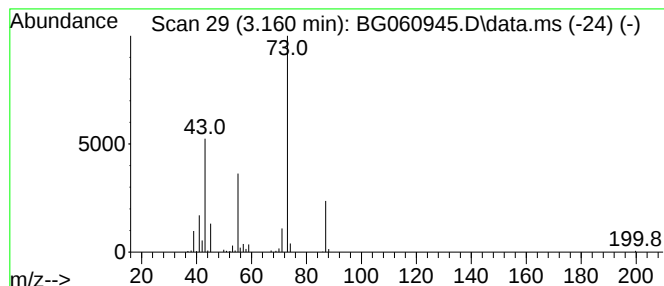
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.160	9.46 ng	150210	1,4-Dichlorobenzene-d4	7.937

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2			Butanoic acid, 2-hydroxy-2-methyl-	132	C6H12O3	032793-34-3	38
3			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	38
4			Silane, tetramethyl-	88	C4H12Si	000075-76-3	32
5			2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	25



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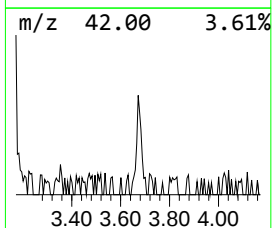
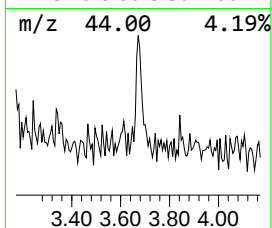
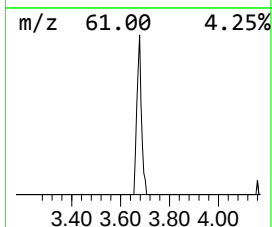
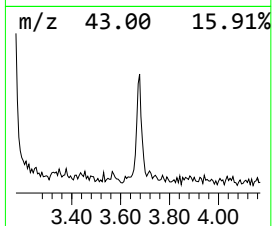
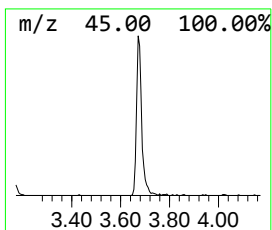
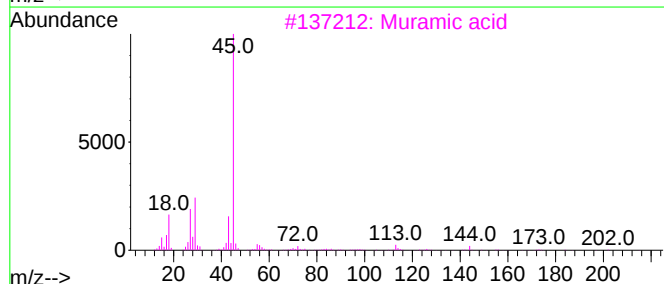
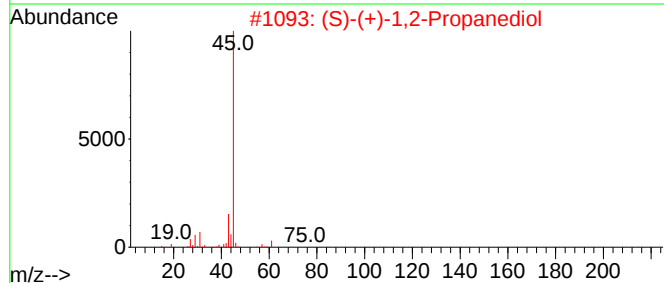
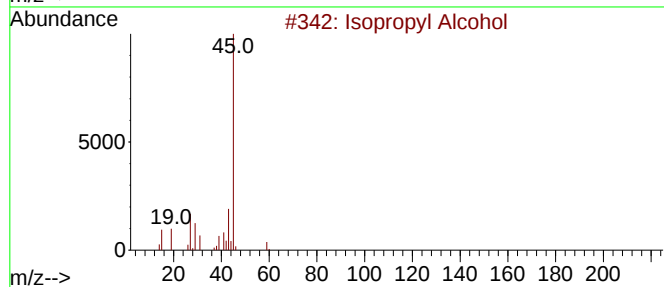
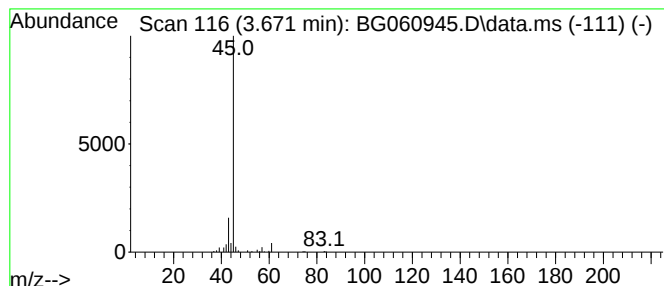
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG041724.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 Isopropyl Alcohol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.671	4.95 ng	78665	1,4-Dichlorobenzene-d4	7.937

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Isopropyl Alcohol	60	C3H8O	000067-63-0	56
2			(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	40
3			Muramic acid	251	C9H17NO7	001114-41-6	9
4			2-Butanol	74	C4H10O	000078-92-2	9
5			Propanoic acid, 2-hydroxy-, meth...	104	C4H8O3	000547-64-8	9



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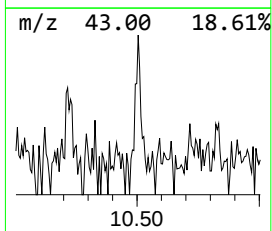
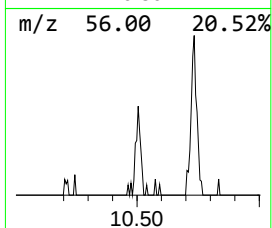
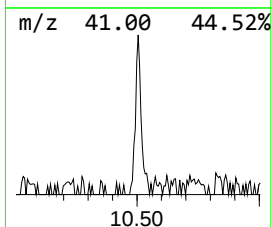
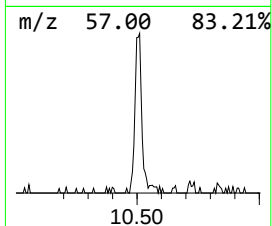
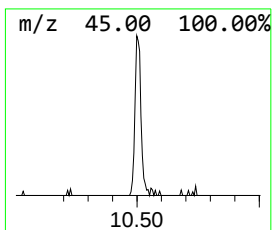
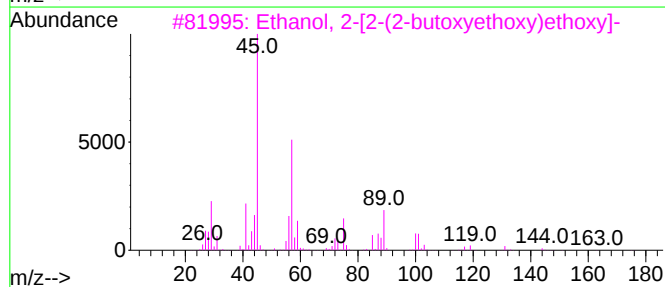
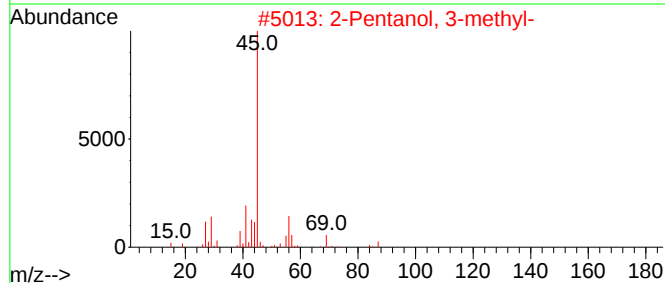
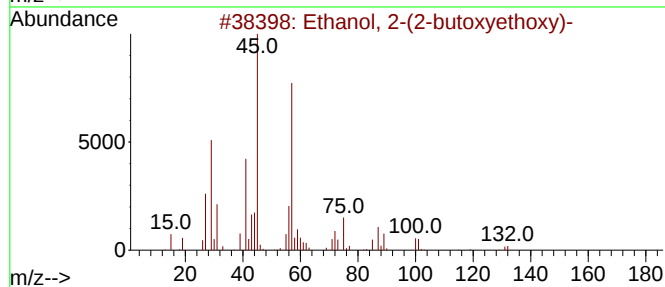
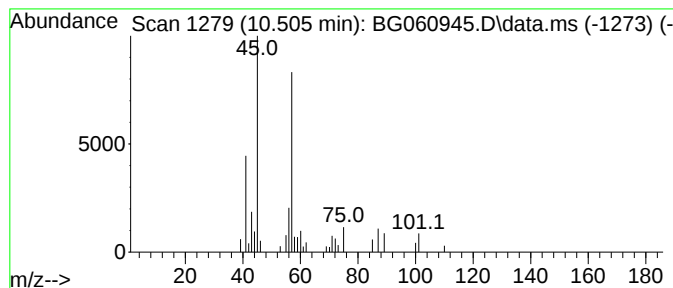
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BNA_G
ClientSampleId :
RPI-SS-DUP-01

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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 3 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.	
10.505	2.15 ng	45848	Naphthalene-d8	10.734	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	78
2	2-Pentanol, 3-methyl-	102	C6H14O	000565-60-6	53
3	Ethanol, 2-[2-(2-butoxyethoxy)et...	206	C10H22O4	000143-22-6	45
4	Propanoic acid, 2-(methoxymethoxy)-	134	C5H10O4	081327-29-9	43
5	Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	42



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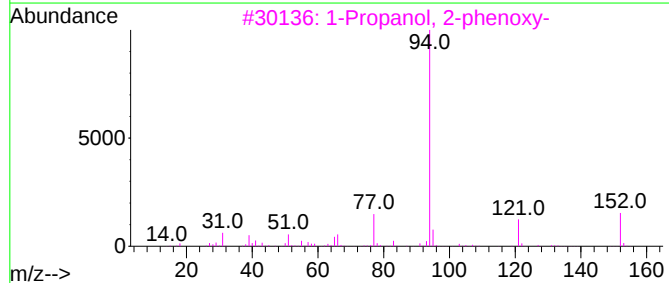
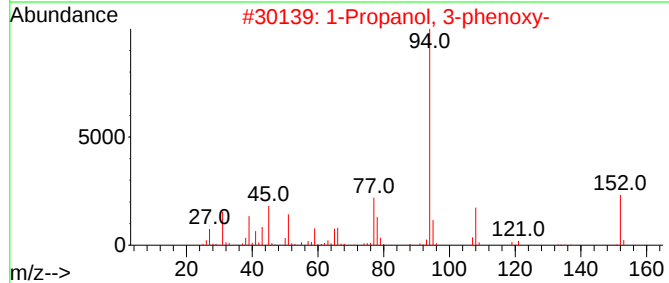
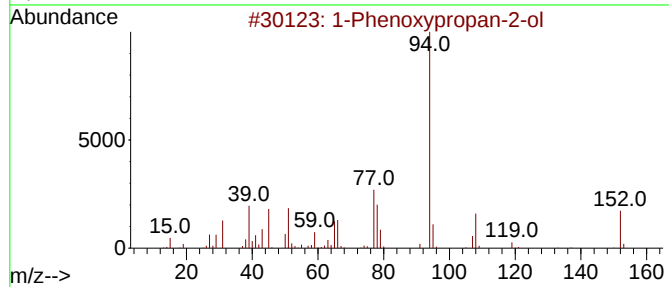
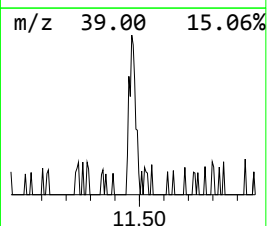
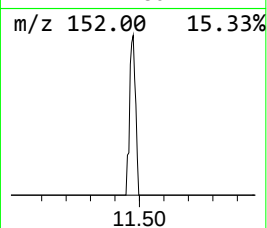
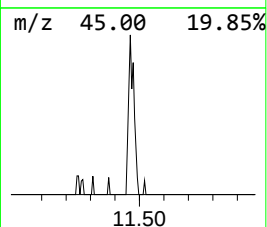
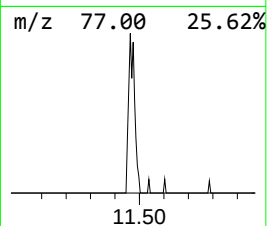
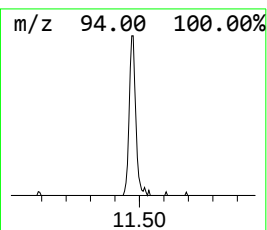
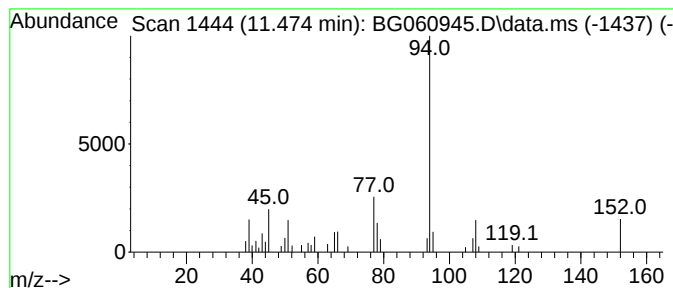
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Peak Number 4 1-Phenoxypropan-2-ol Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.474	2.23 ng	47511	Naphthalene-d8	10.734

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Phenoxypropan-2-ol	152	C9H12O2	000770-35-4	95
2			1-Propanol, 3-phenoxy-	152	C9H12O2	006180-61-6	80
3			1-Propanol, 2-phenoxy-	152	C9H12O2	004169-04-4	53
4			Benzene, (2-methylpropoxy)-	150	C10H14O	001126-75-6	50
5			Pyrimidine, 5-methyl-	94	C5H6N2	002036-41-1	49



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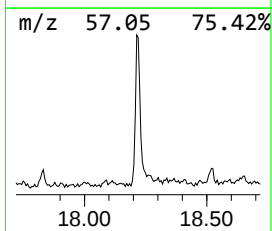
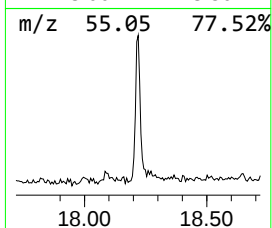
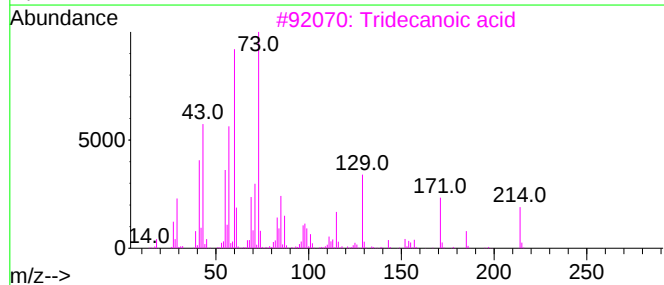
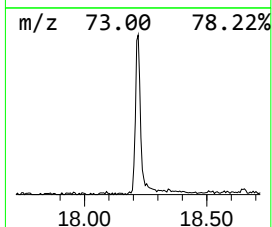
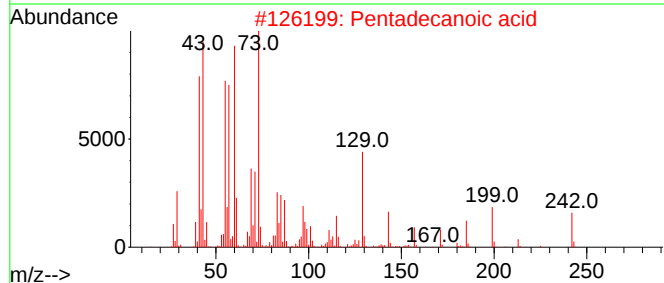
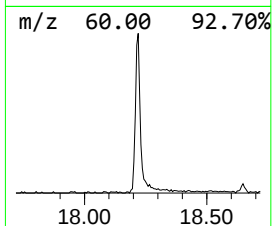
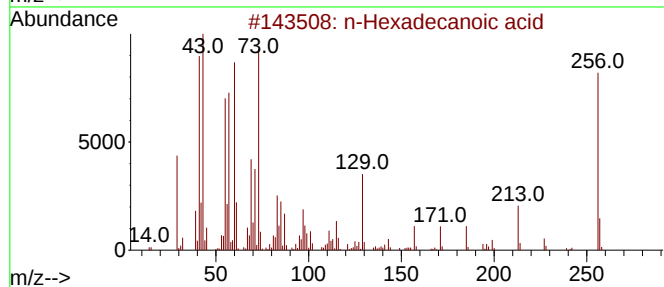
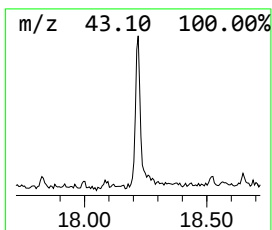
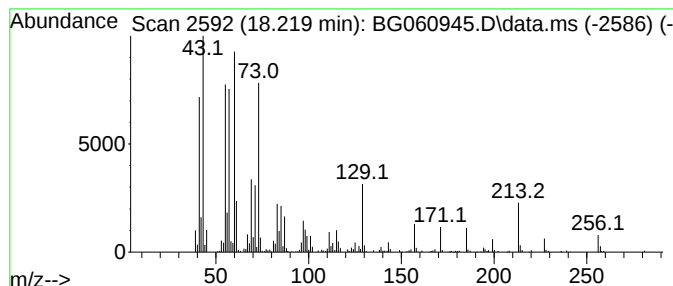
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.219	9.57 ng	483892	Phenanthrene-d10	17.314

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	91
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	81
3			Tridecanoic acid	214	C13H26O2	000638-53-9	58
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	53
5			Dodecanoic acid	200	C12H24O2	000143-07-7	53



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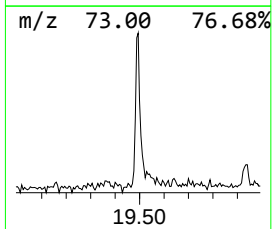
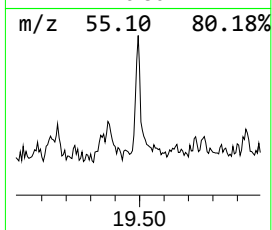
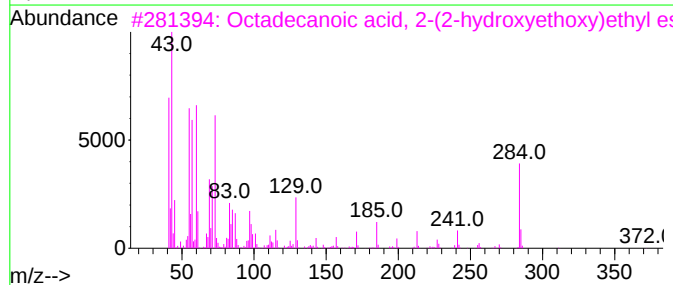
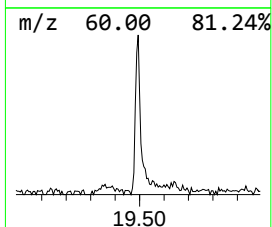
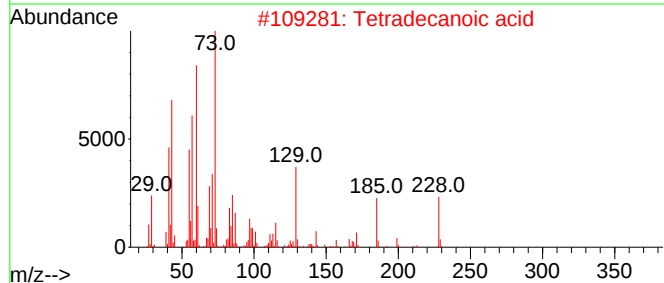
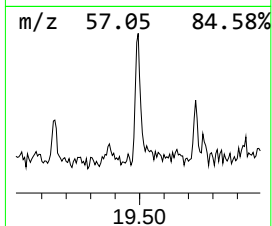
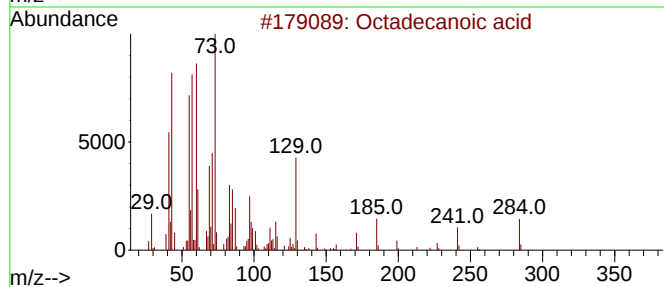
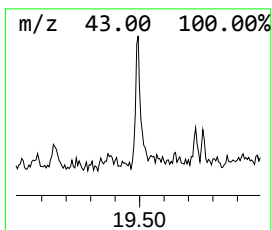
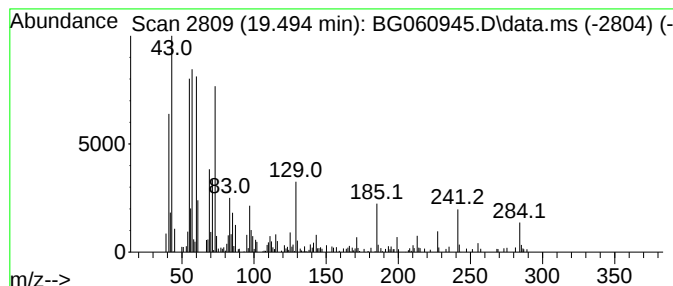
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Octadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.494	3.58 ng	205793	Chrysene-d12	21.568

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	99
2			Tetradecanoic acid	228	C14H28O2	000544-63-8	62
3			Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	59
4			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	53
5			Pentadecanoic acid	242	C15H30O2	001002-84-2	50



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG041824\
Data File : BG060945.D
Acq On : 18 Apr 2024 21:19
Operator : MA/JU
Sample : P2166-03
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
RPI-SS-DUP-01

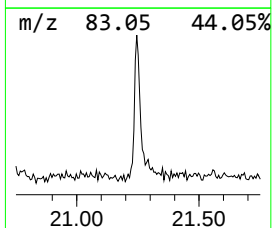
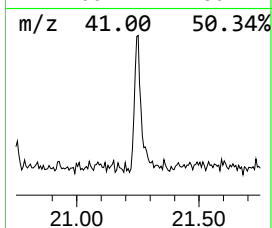
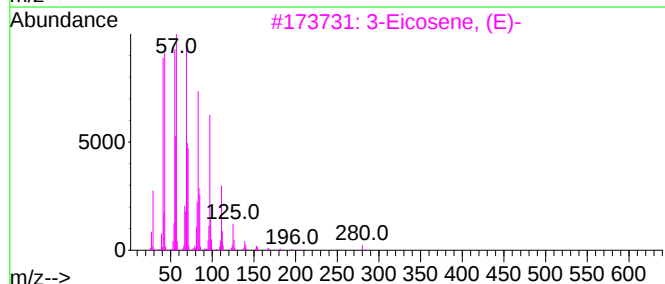
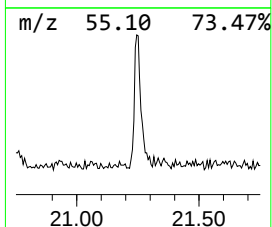
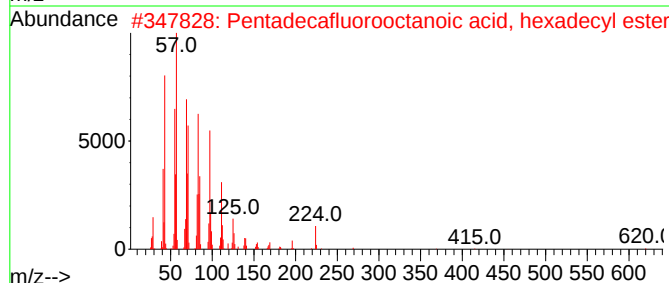
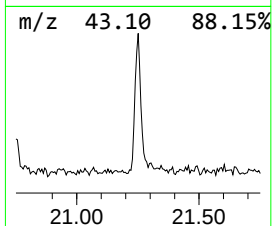
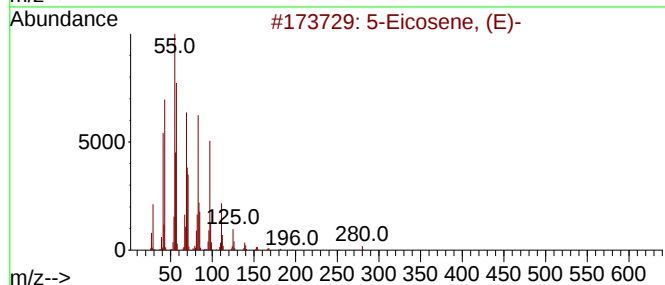
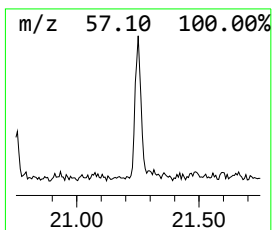
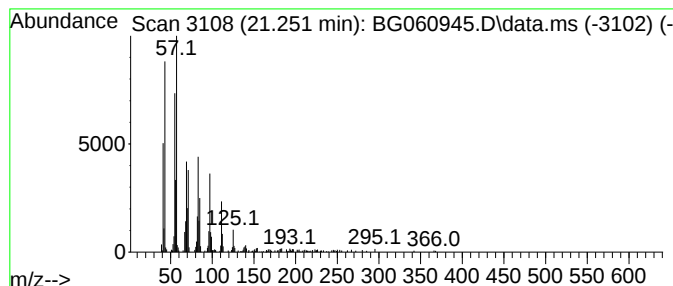
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 5-Eicosene, (E)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.251	6.50 ng	373491	Chrysene-d12	21.568

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			5-Eicosene, (E)-	280	C20H40	074685-30-6	96
2			Pentadecafluorooctanoic acid, he...	638	C24H33F15O2	1000406-04-6	94
3			3-Eicosene, (E)-	280	C20H40	074685-33-9	93
4			Heneicosyl heptafluorobutyrate	508	C25H43F7O2	1000351-83-8	91
5			Octacosyl heptafluorobutyrate	606	C32H57F7O2	1010351-83-6	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG041824\
Data File : BG060945.D
Acq On : 18 Apr 2024 21:19
Operator : MA/JU
Sample : P2166-03
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
RPI-SS-DUP-01

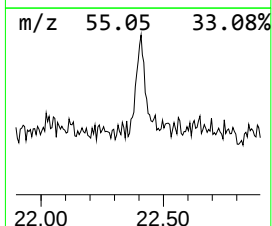
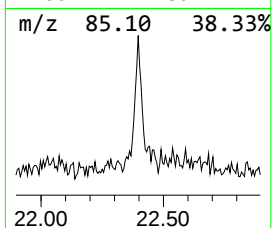
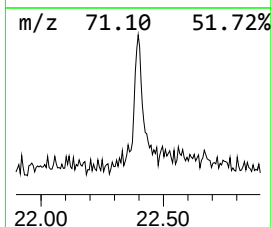
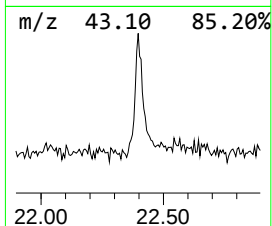
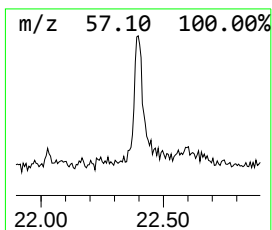
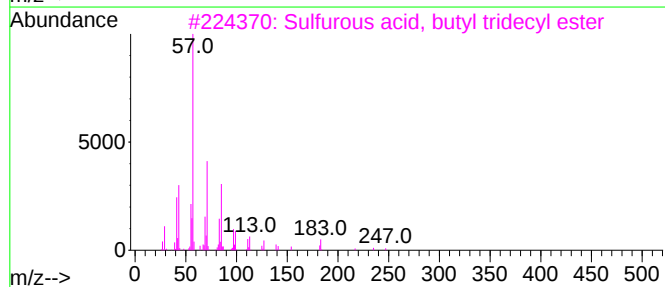
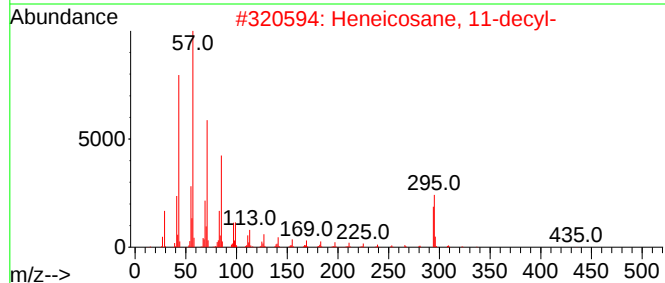
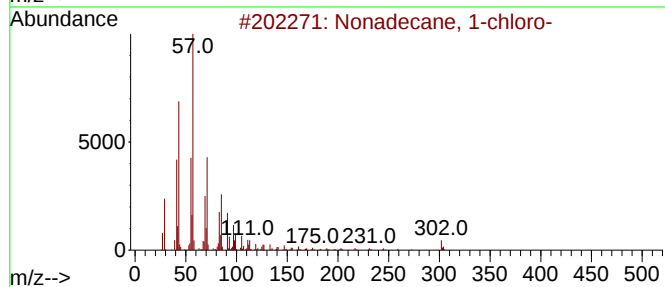
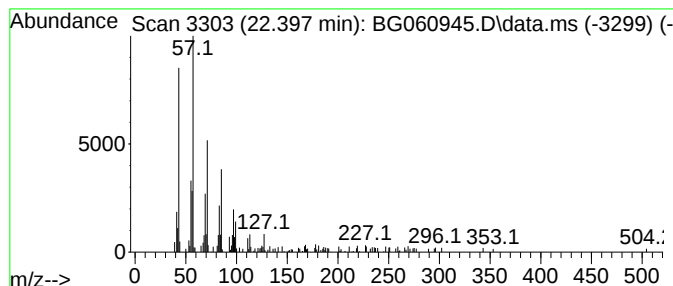
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Nonadecane, 1-chloro- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.397	2.47 ng	142145	Chrysene-d12	21.568

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Nonadecane, 1-chloro-	302	C19H39Cl	062016-76-6	86
2			Heneicosane, 11-decyl-	437	C31H64	055320-06-4	80
3			Sulfurous acid, butyl tridecyl e...	320	C17H36O3S	1000309-18-0	80
4			Tetradecane, 1-chloro-	232	C14H29Cl	002425-54-9	74
5			Heptacosane	380	C27H56	000593-49-7	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG041824\
Data File : BG060945.D
Acq On : 18 Apr 2024 21:19
Operator : MA/JU
Sample : P2166-03
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
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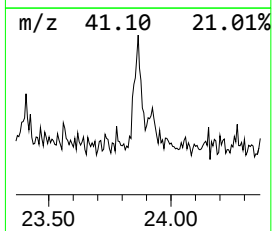
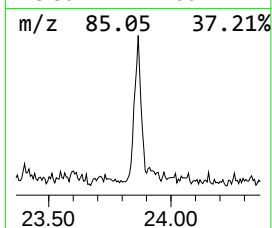
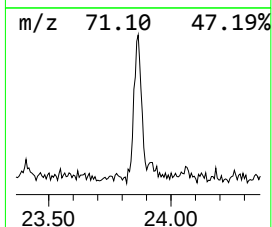
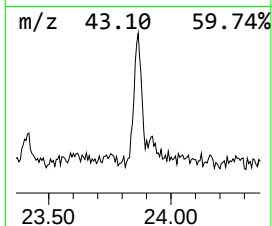
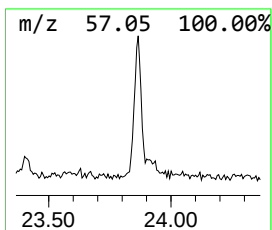
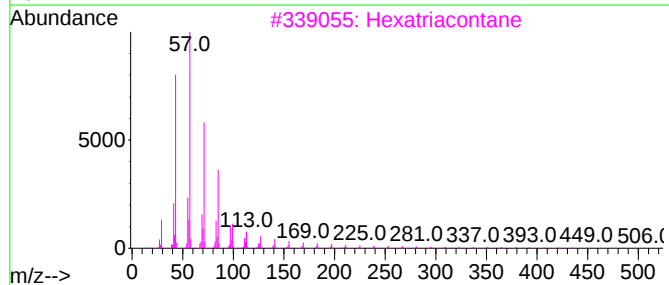
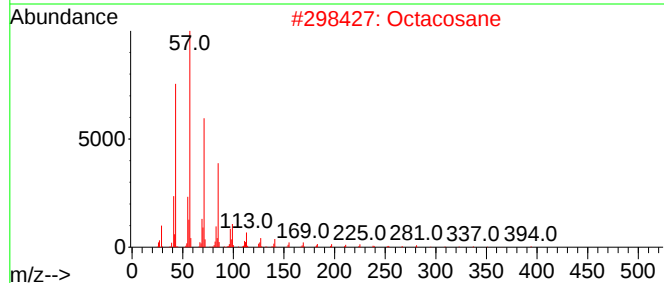
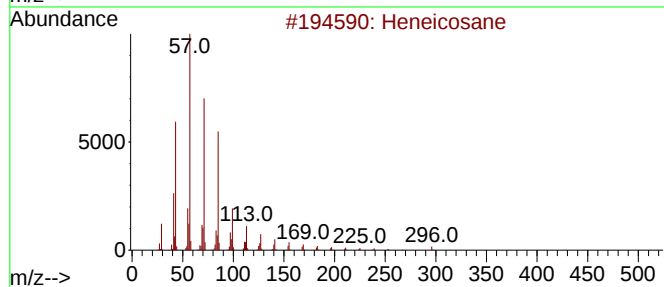
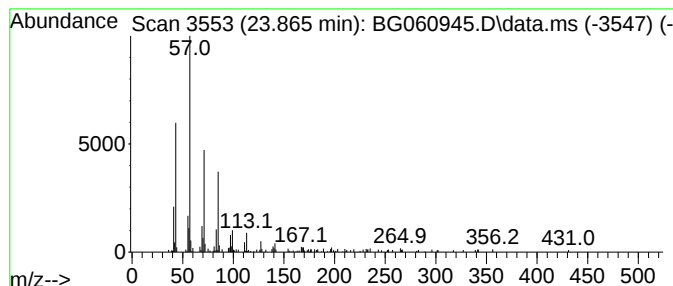
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Heneicosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.865	2.63 ng	163983	Perylene-d12	24.688

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heneicosane	296	C21H44	000629-94-7	94
2			Octacosane	394	C28H58	000630-02-4	87
3			Hexatriacontane	507	C36H74	000630-06-8	83
4			Tetradecane, 1-iodo-	324	C14H29I	019218-94-1	83
5			Docosane, 11-butyl-	366	C26H54	013475-76-8	80



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG041824\
Data File : BG060945.D
Acq On : 18 Apr 2024 21:19
Operator : MA/JU
Sample : P2166-03
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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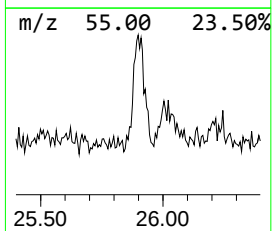
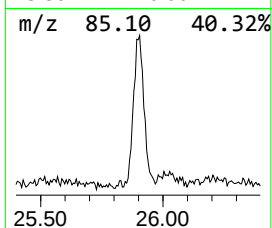
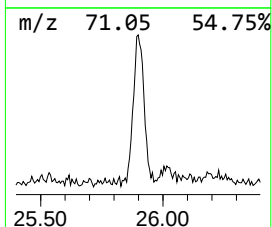
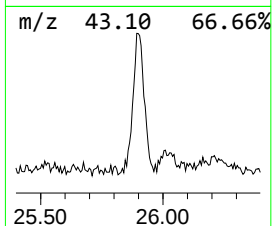
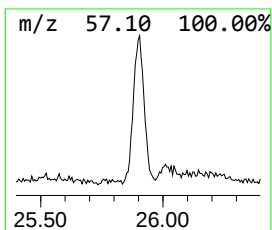
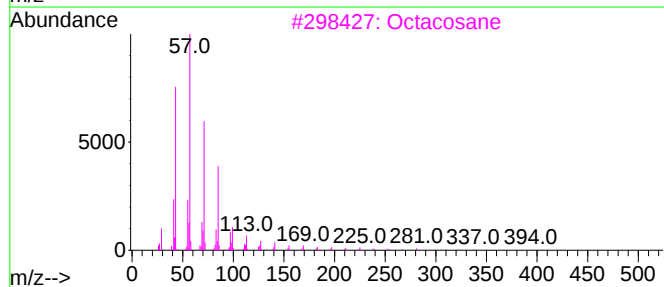
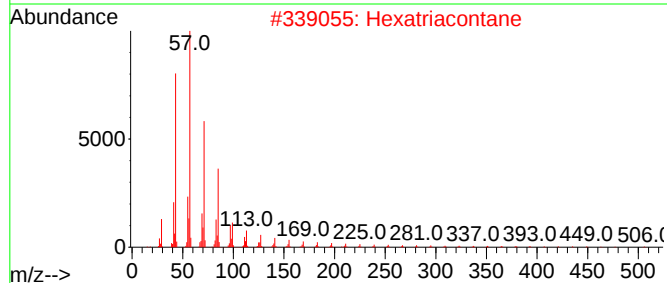
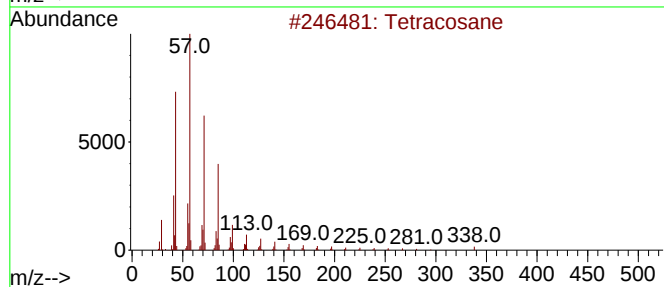
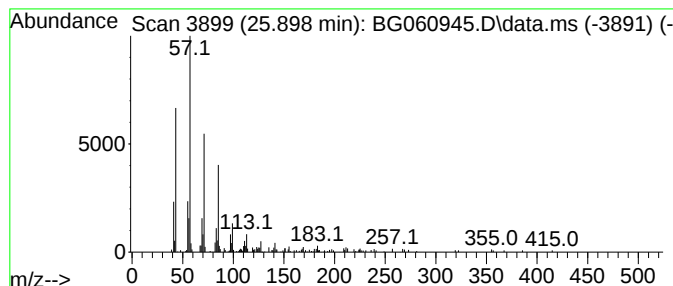
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Tetracosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
25.898	4.69 ng	292411	Perylene-d12	24.688

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Tetracosane	338	C24H50	000646-31-1	87
2		Hexatriacontane	507	C36H74	000630-06-8	87
3		Octacosane	394	C28H58	000630-02-4	87
4		Heneicosane	296	C21H44	000629-94-7	87
5		Octadecane	254	C18H38	000593-45-3	83



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG041824\
Data File : BG060945.D
Acq On : 18 Apr 2024 21:19
Operator : MA/JU
Sample : P2166-03
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
RPI-SS-DUP-01

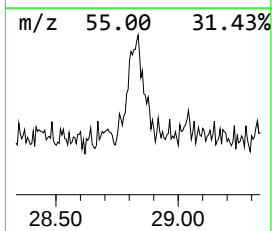
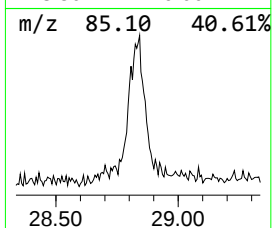
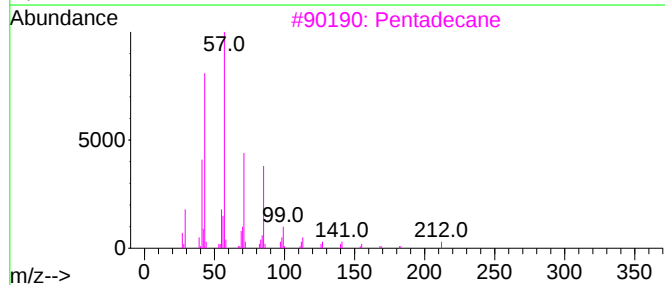
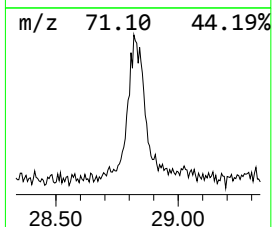
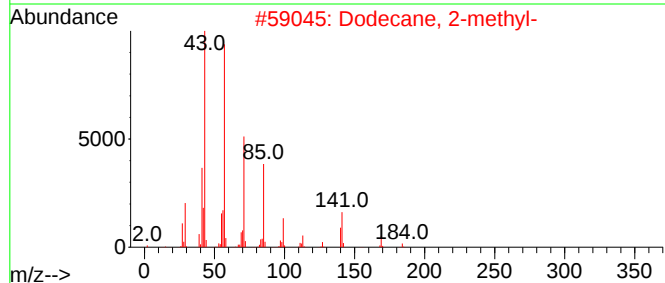
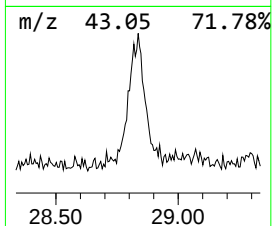
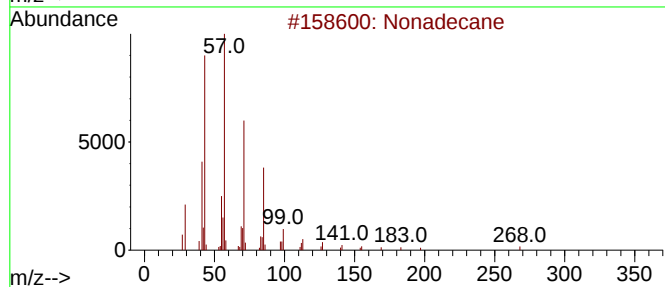
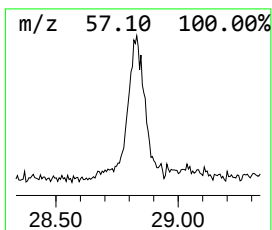
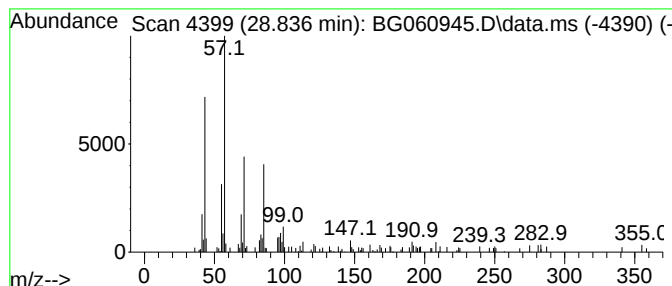
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Nonadecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
28.836	4.12 ng	256972	Perylene-d12	24.688

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Nonadecane	268	C19H40	000629-92-5	87
2			Dodecane, 2-methyl-	184	C13H28	001560-97-0	80
3			Pentadecane	212	C15H32	000629-62-9	72
4			Tridecane	184	C13H28	000629-50-5	58
5			Tricosane, 2-methyl-	338	C24H50	001928-30-9	53



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG041824\
Data File : BG060945.D
Acq On : 18 Apr 2024 21:19
Operator : MA/JU
Sample : P2166-03
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
RPI-SS-DUP-01

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG041724.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
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Isopropyl Alcohol	3.671	5.0	ng	78665	1	7.937	317520	20.0
Ethanol, 2-(2-b...	10.505	2.1	ng	45848	2	10.734	425848	20.0
1-Phenoxypropan...	11.474	2.2	ng	47511	2	10.734	425848	20.0
n-Hexadecanoic ...	18.219	9.6	ng	483892	4	17.314	1011400	20.0
Octadecanoic acid	19.494	3.6	ng	205793	5	21.568	1149790	20.0
5-Eicosene, (E)-	21.251	6.5	ng	373491	5	21.568	1149790	20.0
Nonadecane, 1-c...	22.397	2.5	ng	142145	5	21.568	1149790	20.0
Heneicosane	23.865	2.6	ng	163983	6	24.688	1247180	20.0
Tetracosane	25.898	4.7	ng	292411	6	24.688	1247180	20.0
Nonadecane	28.836	4.1	ng	256972	6	24.688	1247180	20.0