

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF070324\
 Data File : BF138447.D
 Acq On : 03 Jul 2024 15:42
 Operator : CG\JU
 Sample : P3141-02
 Misc :
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 B-140-SB01

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_F\Methods\8270-BF062824.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF138447.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.187	10	17	23	rVB	2489335	3126246	85.37%	11.389%
2	2.293	29	35	42	rBV	42345	53758	1.47%	0.196%
3	3.410	221	225	238	rBV	78050	153110	4.18%	0.558%
4	5.092	507	511	521	rVB	390114	459514	12.55%	1.674%
5	5.498	576	580	583	rBV	3586996	3400083	92.85%	12.386%
6	6.504	746	751	754	rBV	3651992	3560319	97.23%	12.970%
7	6.869	809	813	817	rVB	1121043	898171	24.53%	3.272%
8	7.433	903	909	912	rBV	2390834	2308796	63.05%	8.411%
9	7.680	948	951	955	rBV	99706	84406	2.30%	0.307%
10	8.151	1024	1031	1034	rBV	1206115	1013525	27.68%	3.692%
11	8.457	1075	1083	1087	rBV	122509	134558	3.67%	0.490%
12	9.227	1208	1214	1217	rBV	4278334	3661919	100.00%	13.340%
13	9.904	1325	1329	1332	rBV	1312974	1020880	27.88%	3.719%
14	9.998	1339	1345	1351	rBV2	79485	110910	3.03%	0.404%
15	10.692	1459	1463	1466	rBV	1853546	1533611	41.88%	5.587%
16	11.392	1578	1582	1584	rBV	936040	821671	22.44%	2.993%
17	11.410	1584	1585	1589	rVB	129275	92727	2.53%	0.338%
18	11.916	1668	1671	1678	rBV2	151723	151095	4.13%	0.550%
19	12.598	1784	1787	1791	rBV	144798	124214	3.39%	0.452%
20	12.698	1801	1804	1812	rBV5	37435	53340	1.46%	0.194%
21	12.827	1821	1826	1832	rVB	130862	146378	4.00%	0.533%
22	12.974	1847	1851	1854	rBV	2369114	2026244	55.33%	7.381%
23	13.204	1885	1890	1892	rBV	57850	57435	1.57%	0.209%
24	13.545	1944	1948	1951	rBV	135671	118900	3.25%	0.433%
25	13.874	2000	2004	2013	rBV	266662	307086	8.39%	1.119%
26	14.027	2025	2030	2033	rBV	644033	646170	17.65%	2.354%
27	14.186	2054	2057	2063	rBV	223957	199070	5.44%	0.725%
28	14.492	2105	2109	2114	rBV	214429	197567	5.40%	0.720%
29	14.798	2157	2161	2165	rBV	148781	149147	4.07%	0.543%
30	15.062	2201	2206	2209	rBV2	39378	61673	1.68%	0.225%
31	15.139	2215	2219	2229	rVB	98182	121017	3.30%	0.441%
32	15.368	2254	2258	2264	rBV3	28210	42941	1.17%	0.156%
33	15.427	2264	2268	2274	rVB	35382	49063	1.34%	0.179%
34	15.492	2274	2279	2283	rBV	395752	501718	13.70%	1.828%
35	15.521	2283	2284	2293	rVB2	68344	63636	1.74%	0.232%

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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_F\Methods\8270-BF062824.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

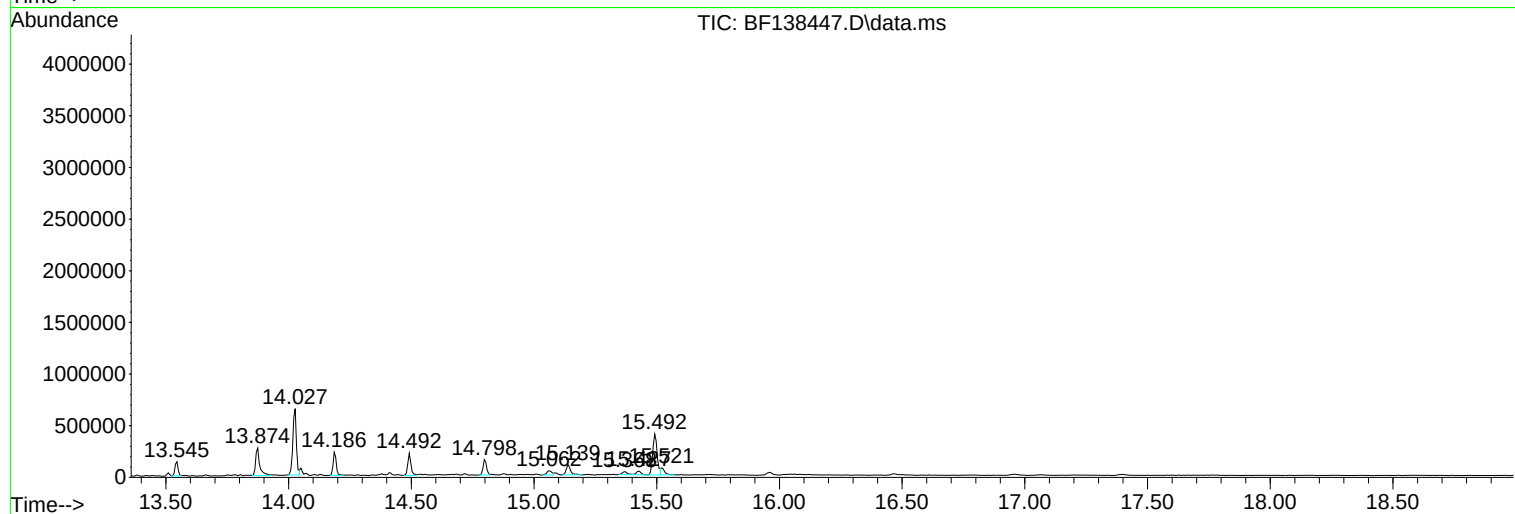
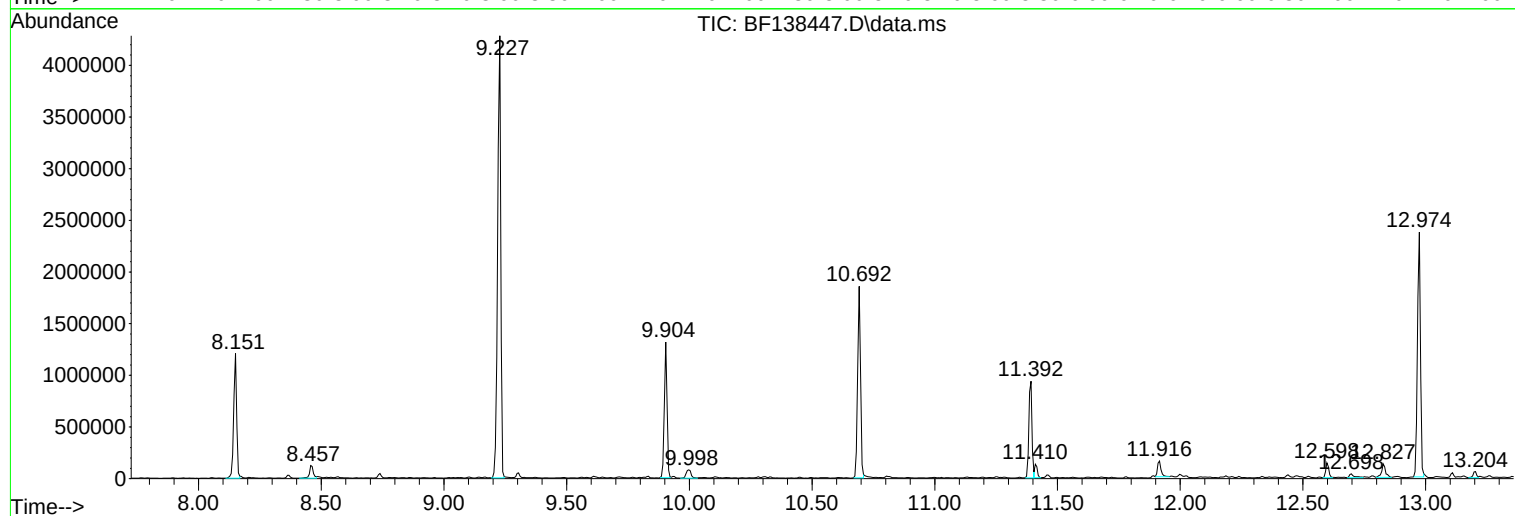
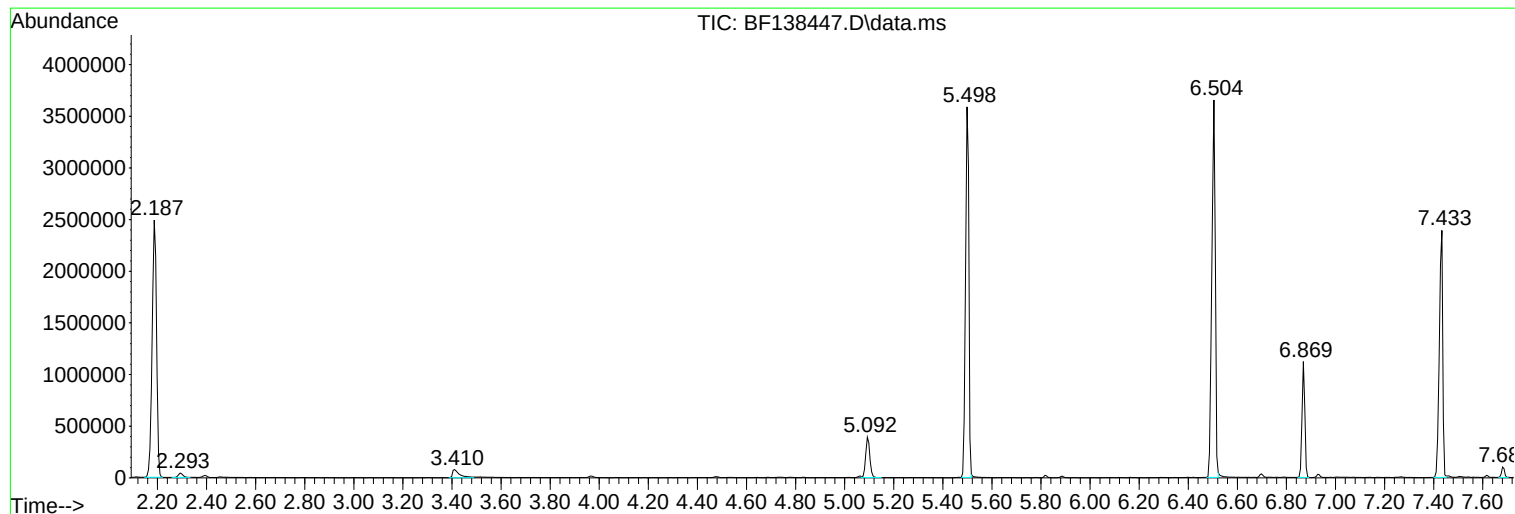
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062824.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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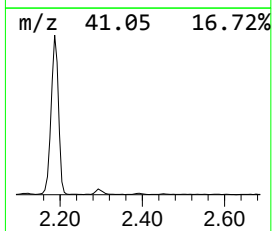
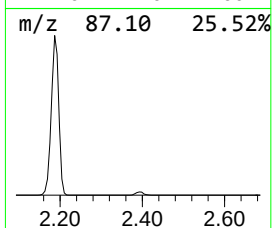
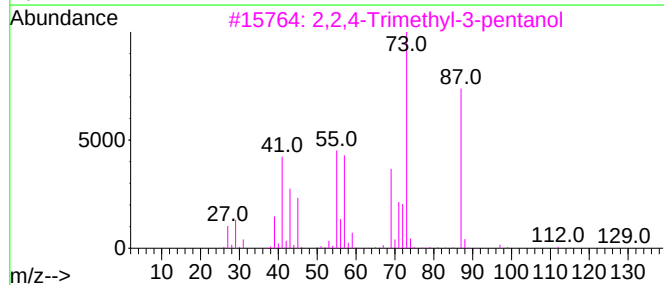
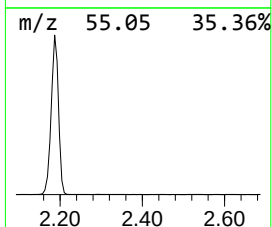
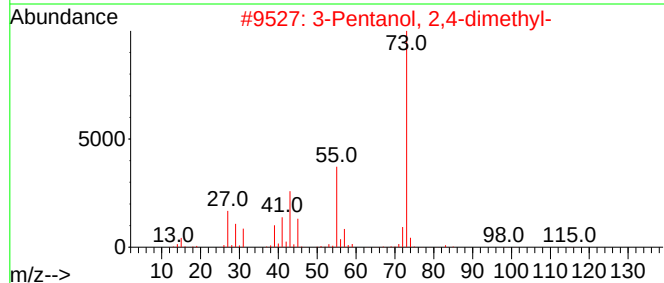
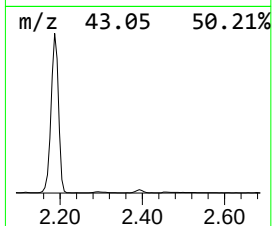
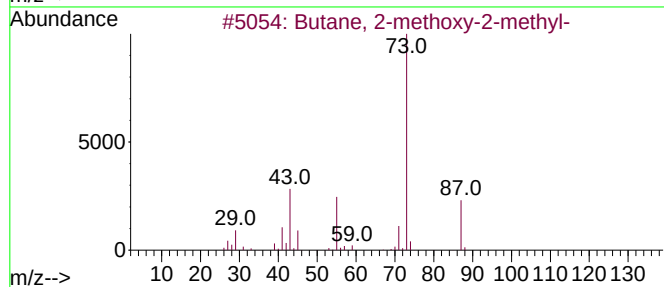
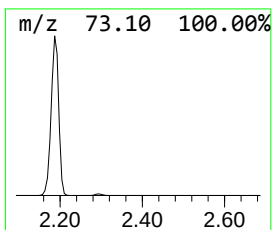
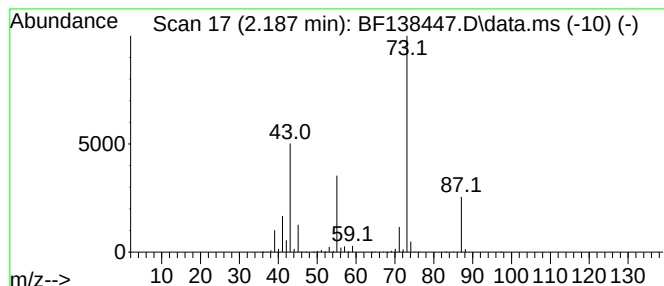
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062824.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.187	69.61 ng	3126250	1,4-Dichlorobenzene-d4	6.869

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2			3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	43
3			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
4			Silane, tetramethyl-	88	C4H12Si	000075-76-3	38
5			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	23



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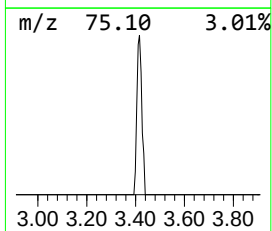
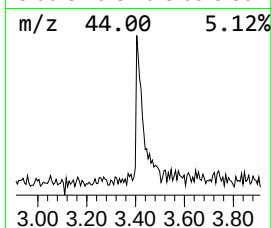
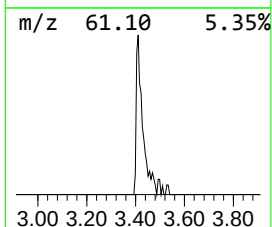
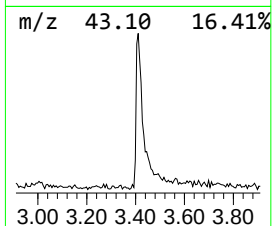
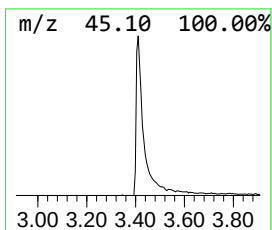
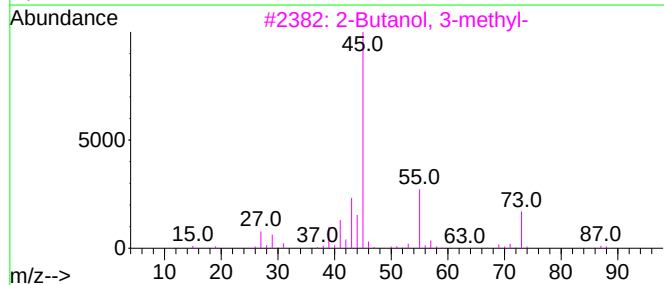
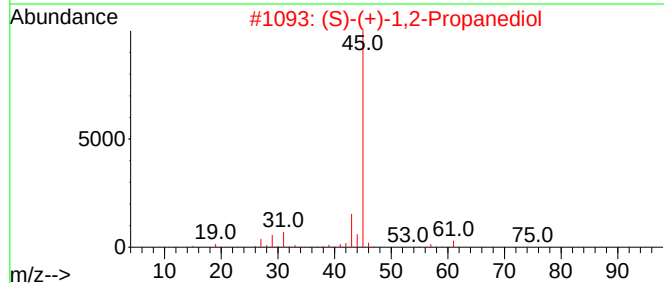
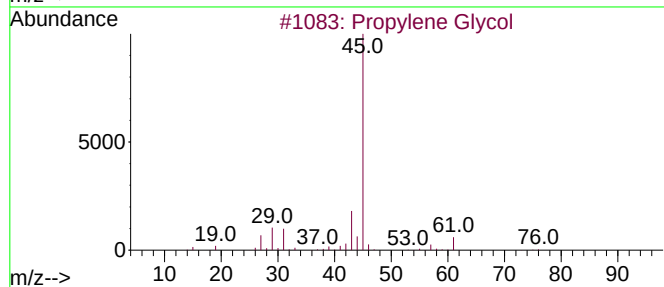
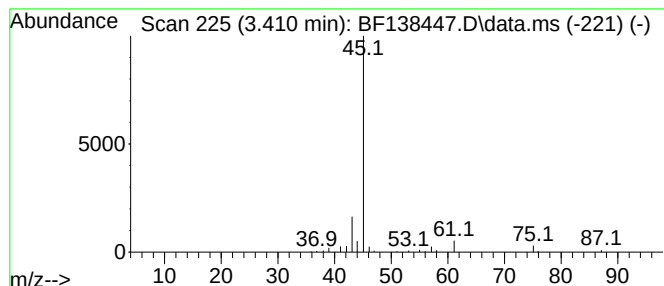
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062824.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Propylene Glycol Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.410	3.41 ng	153110	1,4-Dichlorobenzene-d4	6.869

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propylene Glycol	76	C3H8O2	000057-55-6	78
2			(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	56
3			2-Butanol, 3-methyl-	88	C5H12O	000598-75-4	39
4			R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	32
5			Propanoic acid, 2-hydroxy-, meth...	104	C4H8O3	000547-64-8	9



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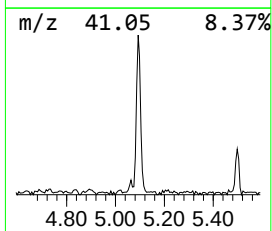
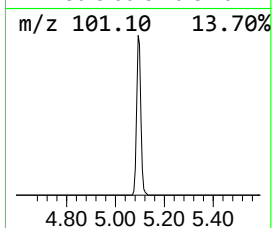
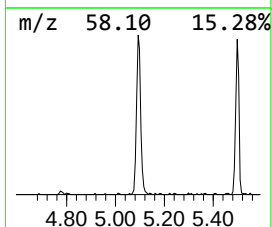
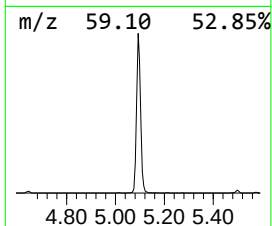
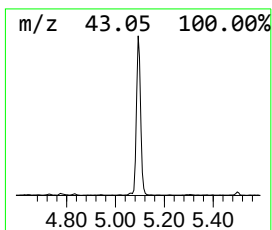
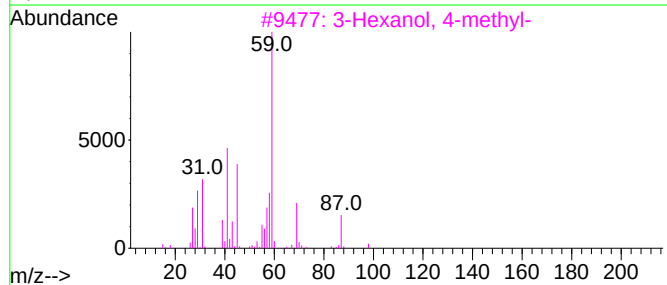
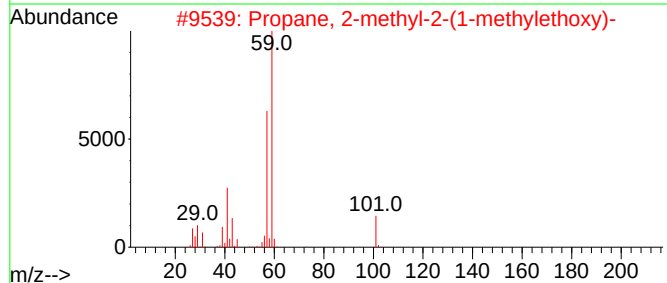
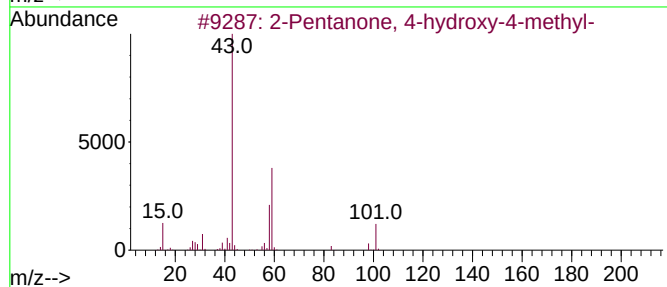
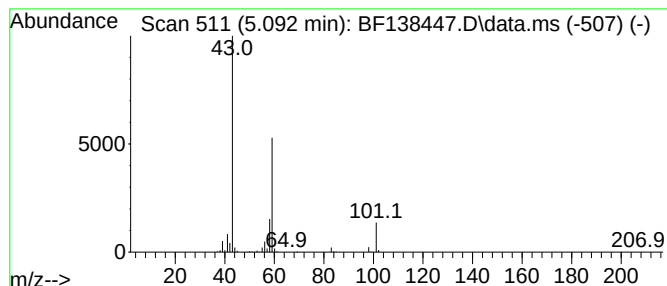
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.092	10.23 ng	459514	1,4-Dichlorobenzene-d4	6.869

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2			Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36
3			3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	27
5			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25



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Instrument :
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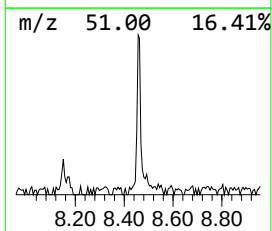
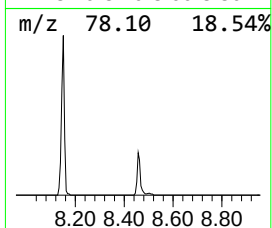
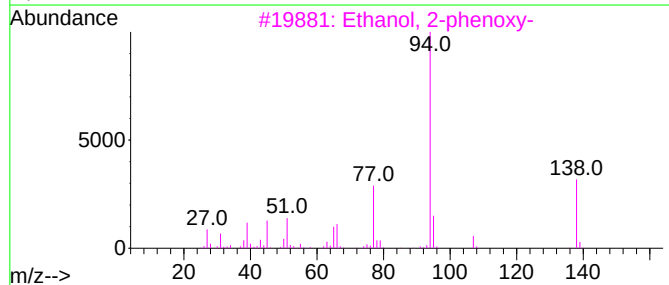
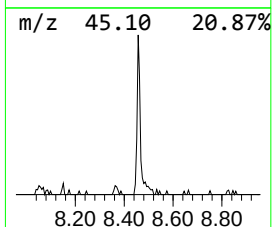
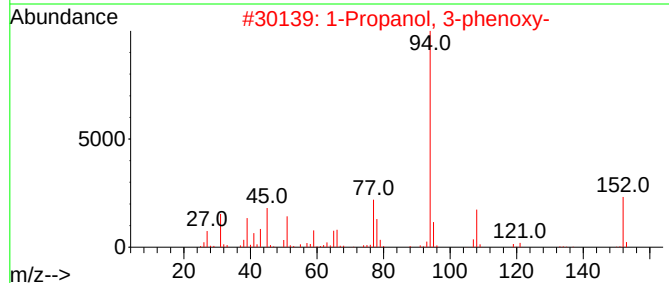
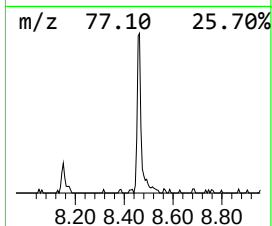
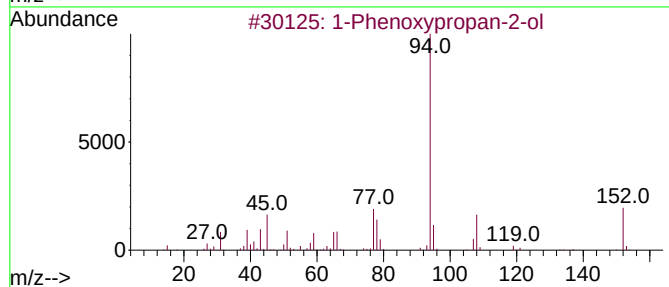
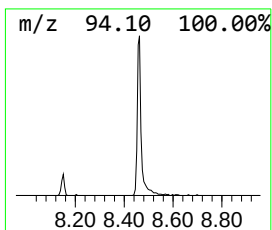
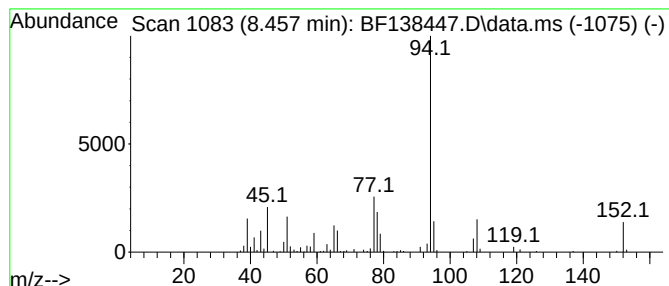
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 1-Phenoxypropan-2-ol Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.457	2.66 ng	134558	Naphthalene-d8	8.151

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	78
3			Ethanol, 2-phenoxy-	138	C8H10O2	000122-99-6	64
4			Benzene, (2-methylpropoxy)-	150	C10H14O	001126-75-6	50
5			1-Propanol, 2-phenoxy-	152	C9H12O2	004169-04-4	50



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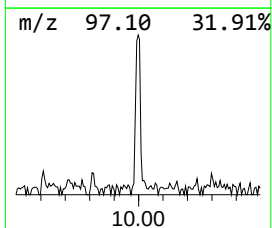
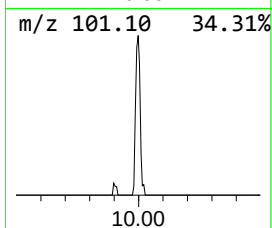
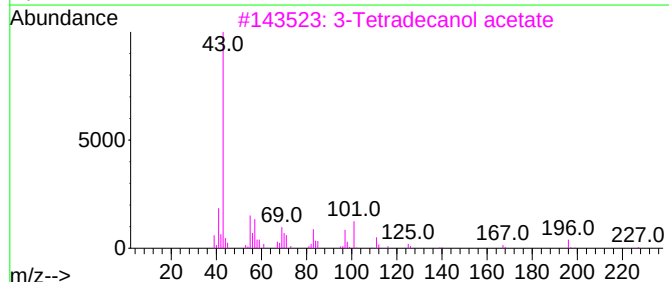
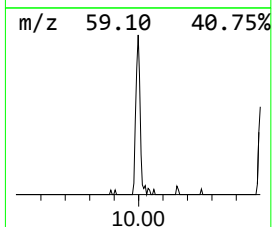
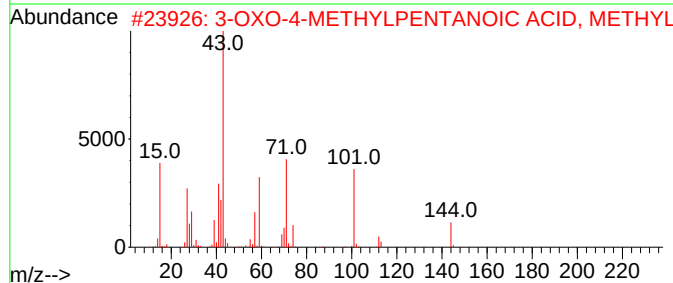
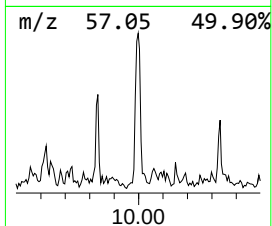
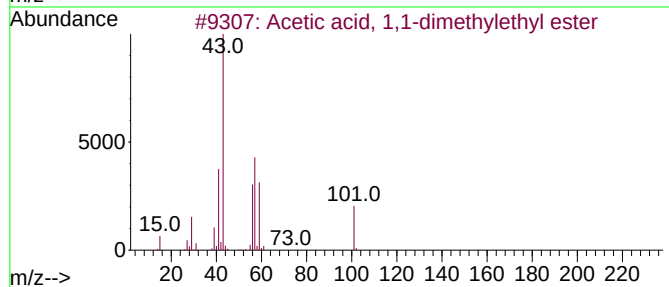
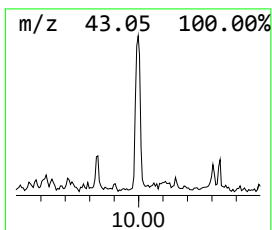
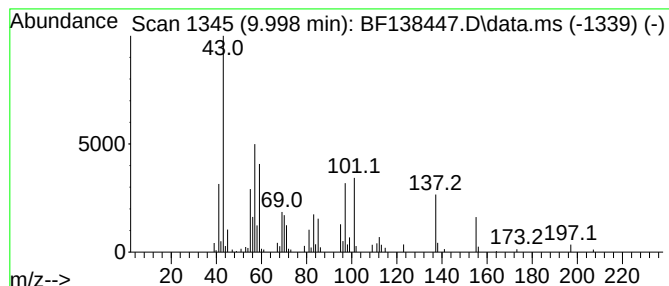
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 unknown9.998 Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.998	2.17 ng	110910	Acenaphthene-d10	9.904

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	16
2			3-OXO-4-METHYLPENTANOIC ACID, ME...	144	C7H12O3	042558-54-3	16
3			3-Tetradecanol acetate	256	C16H32O2	051354-23-5	12
4			Acetamide, N-(aminocarbonyl)-	102	C3H6N2O2	000591-07-1	10
5			2-Hexanone, 4-methyl-	114	C7H14O	000105-42-0	10



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Acq On : 03 Jul 2024 15:42
Operator : CG\JU
Sample : P3141-02
Misc :
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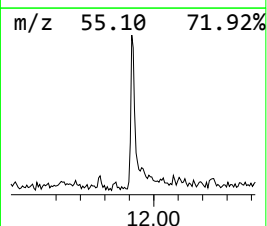
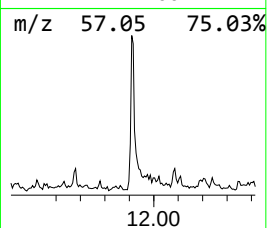
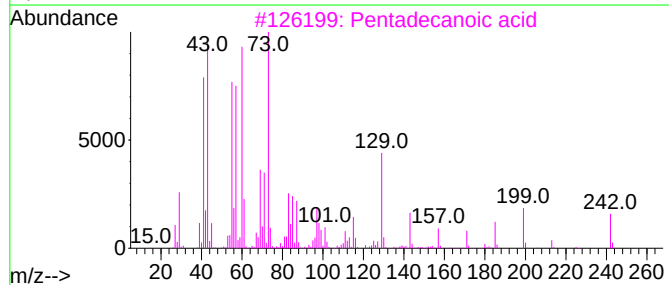
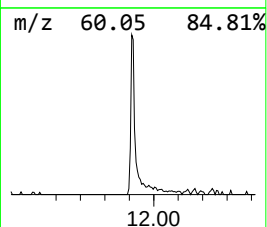
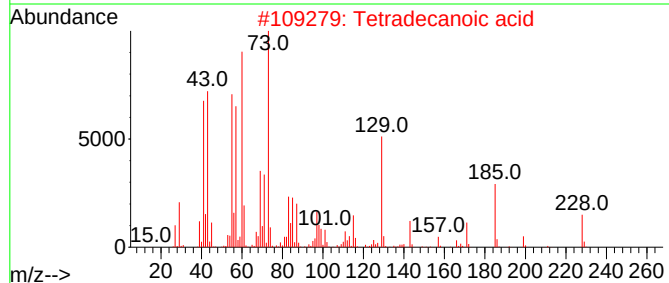
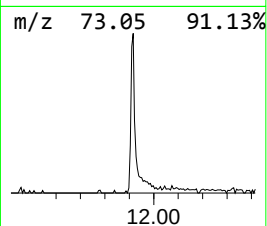
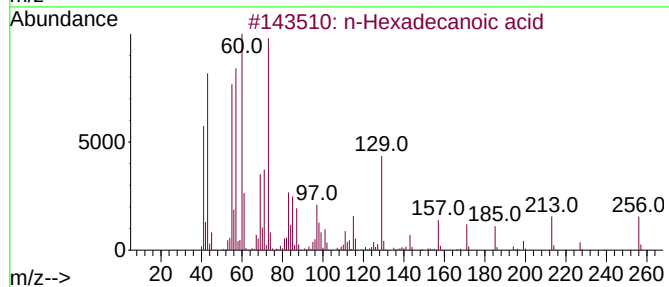
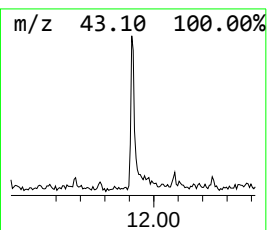
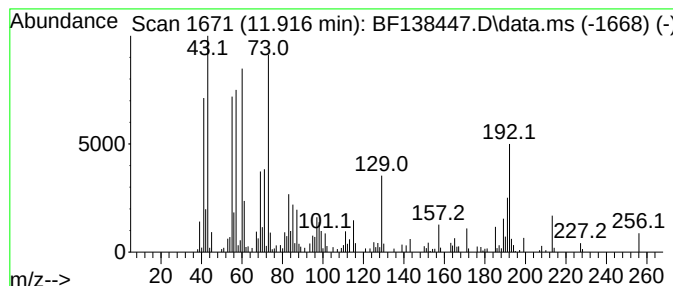
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 n-Hexadecanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD		R.T.	
11.916	3.68 ng	151095	Phenanthrene-d10		11.392	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid		256	C16H32O2	000057-10-3	99
2	Tetradecanoic acid		228	C14H28O2	000544-63-8	91
3	Pentadecanoic acid		242	C15H30O2	001002-84-2	76
4	n-Decanoic acid		172	C10H20O2	000334-48-5	64
5	Undecanoic acid		186	C11H22O2	000112-37-8	62



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF070324\
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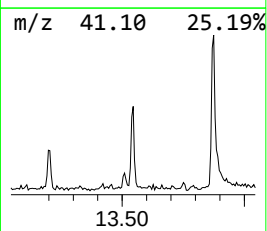
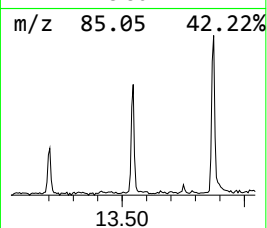
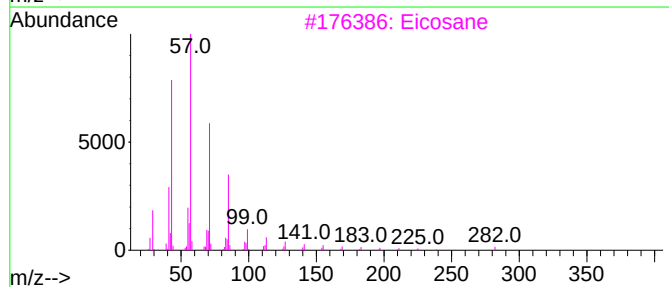
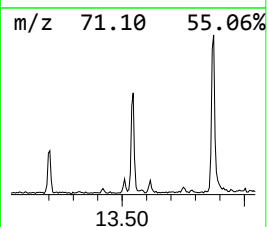
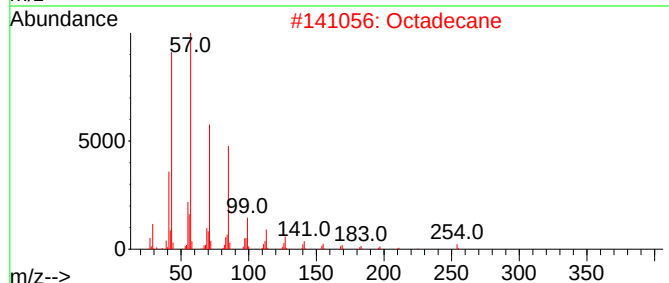
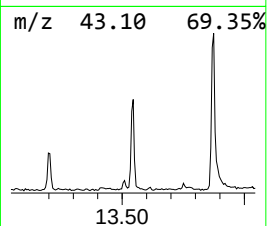
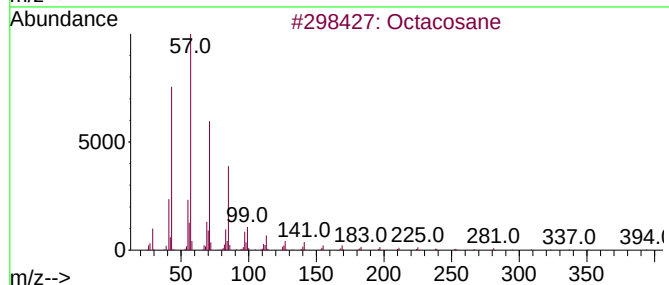
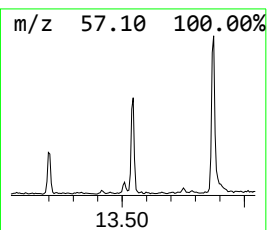
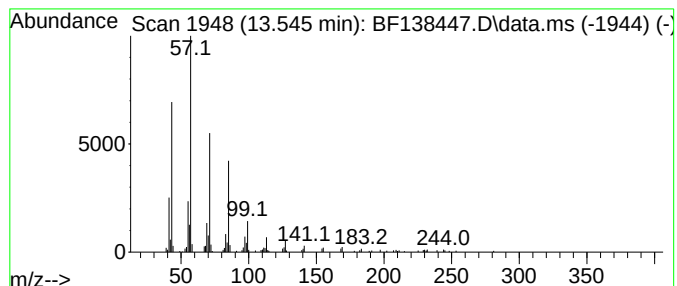
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Octacosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.545	3.68 ng	118900	Chrysene-d12	14.027

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octacosane	394	C28H58	000630-02-4	91
2			Octadecane	254	C18H38	000593-45-3	91
3			Eicosane	282	C20H42	000112-95-8	90
4			Docosane	310	C22H46	000629-97-0	90
5			Heneicosane	296	C21H44	000629-94-7	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF070324\
Data File : BF138447.D
Acq On : 03 Jul 2024 15:42
Operator : CG\JU
Sample : P3141-02
Misc :
ALS Vial : 11 Sample Multiplier: 1

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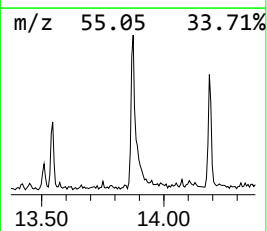
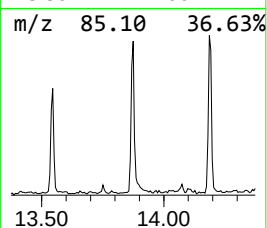
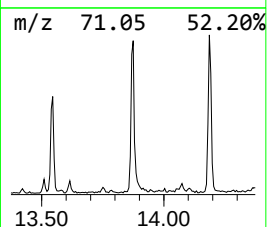
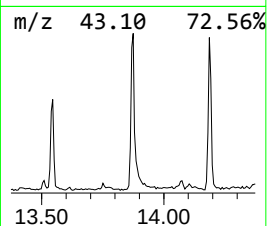
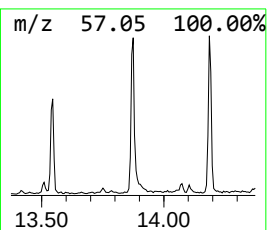
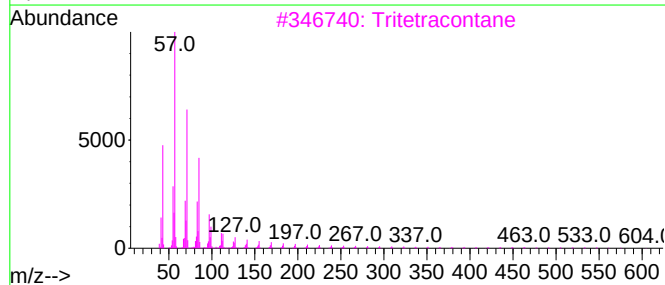
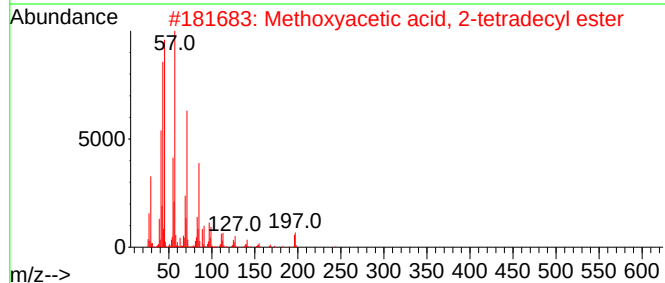
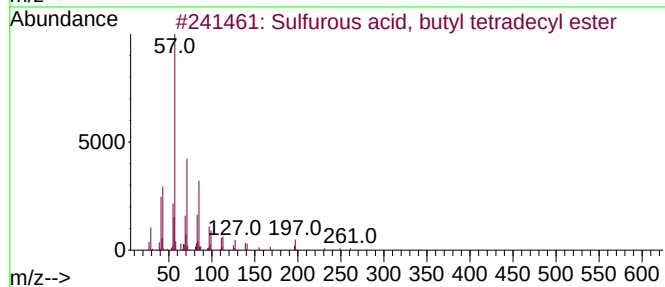
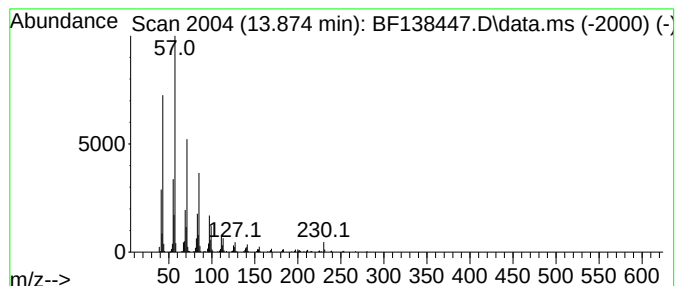
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Sulfurous acid, butyl tetra... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.874	9.50 ng	307086	Chrysene-d12	14.027

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfurous acid, butyl tetradecyl...	334	C18H38O3S	1010309-18-1	91
2			Methoxyacetic acid, 2-tetradecyl...	286	C17H34O3	1000282-04-8	91
3			Tritetracontane	605	C43H88	007098-21-7	91
4			Heptacosane, 1-chloro-	414	C27H55Cl	062016-79-9	87
5			Eicosane	282	C20H42	000112-95-8	83



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF070324\
Data File : BF138447.D
Acq On : 03 Jul 2024 15:42
Operator : CG\JU
Sample : P3141-02
Misc :
ALS Vial : 11 Sample Multiplier: 1

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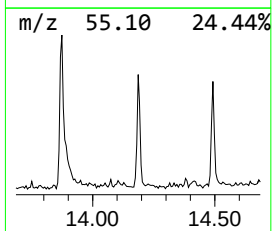
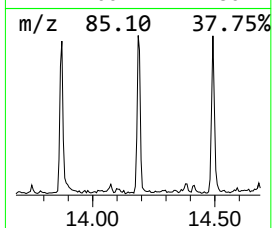
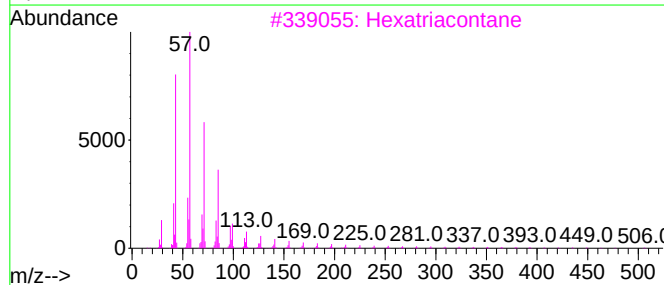
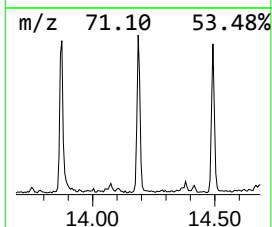
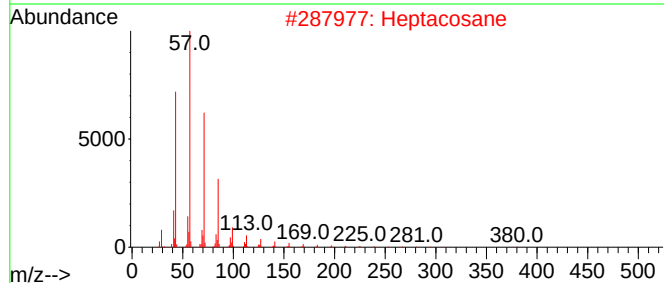
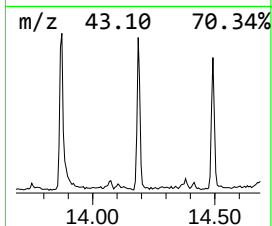
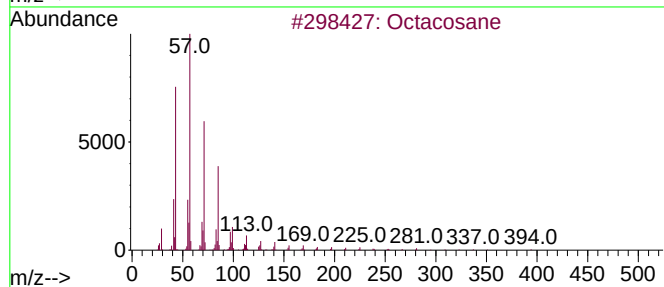
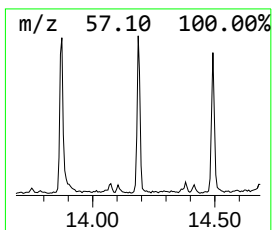
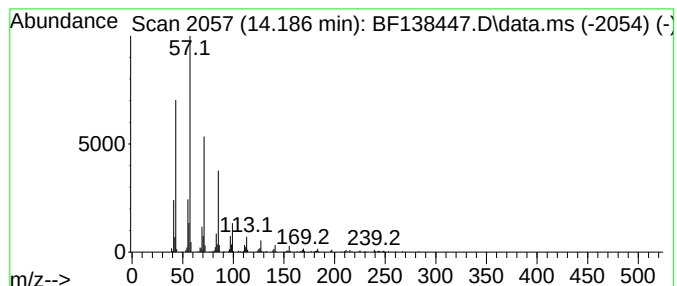
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Heptacosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.186	6.16 ng	199070	Chrysene-d12	14.027

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Octacosane	394	C28H58	000630-02-4	91
2		Heptacosane	380	C27H56	000593-49-7	91
3		Hexatriacontane	507	C36H74	000630-06-8	91
4		Tetracosane	338	C24H50	000646-31-1	90
5		Eicosane, 7-hexyl-	366	C26H54	055333-99-8	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF070324\
Data File : BF138447.D
Acq On : 03 Jul 2024 15:42
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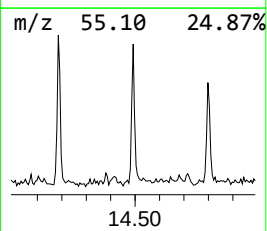
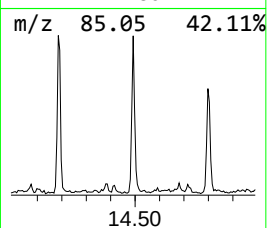
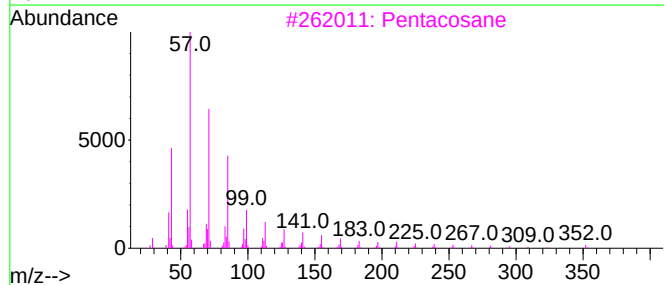
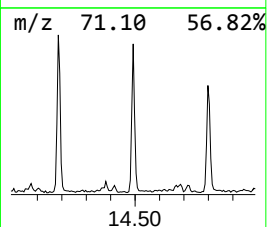
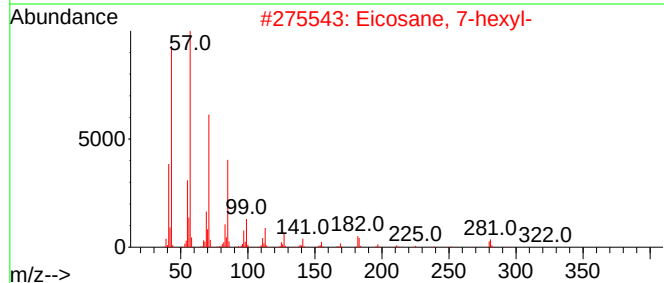
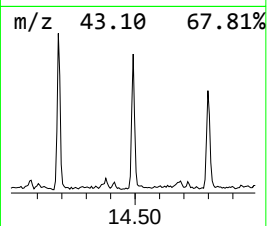
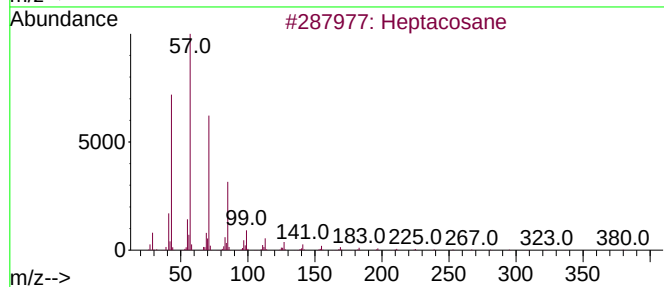
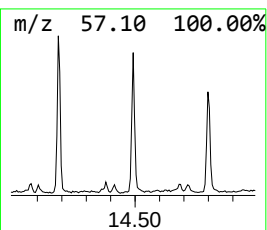
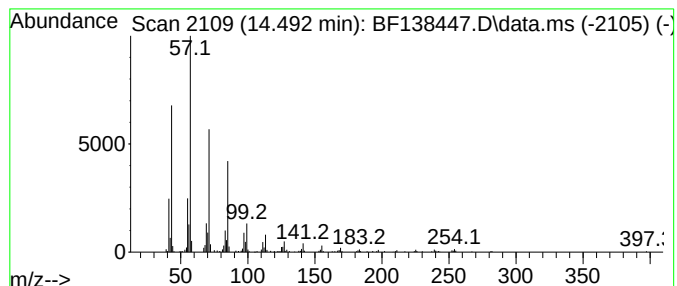
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Eicosane, 7-hexyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.492	6.12 ng	197567	Chrysene-d12	14.027

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Heptacosane	380	C27H56	000593-49-7	91
2		Eicosane, 7-hexyl-	366	C26H54	055333-99-8	91
3		Pentacosane	352	C25H52	000629-99-2	91
4		Docosane, 11-butyl-	366	C26H54	013475-76-8	91
5		Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF070324\
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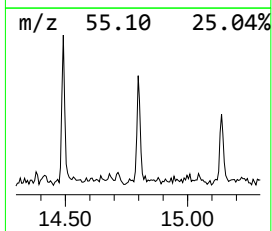
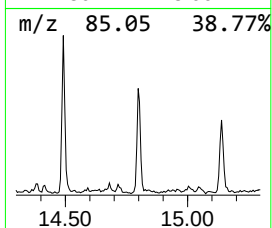
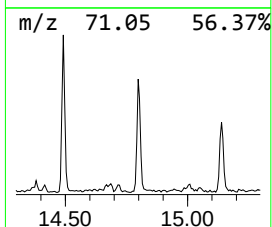
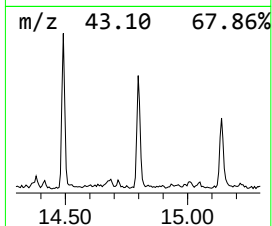
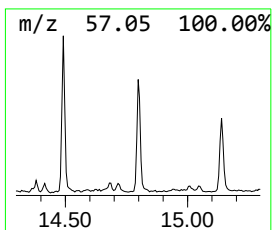
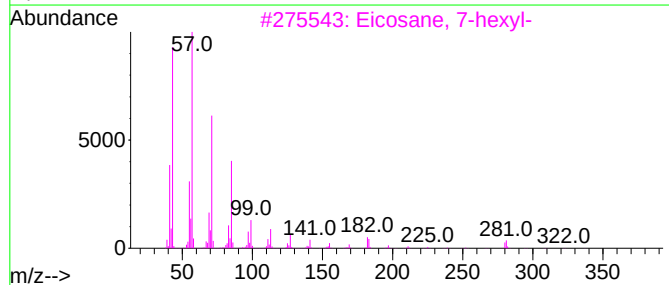
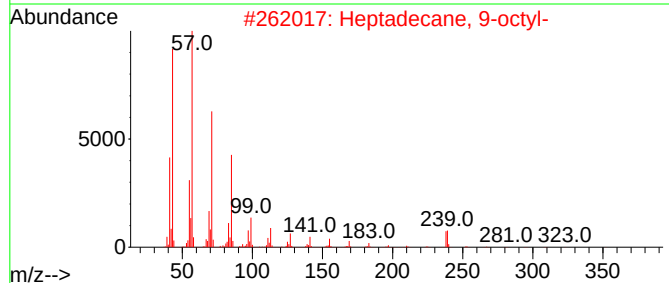
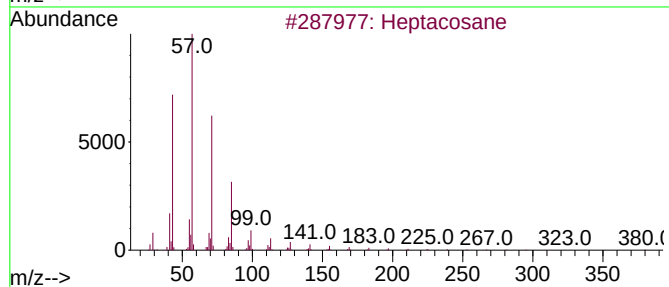
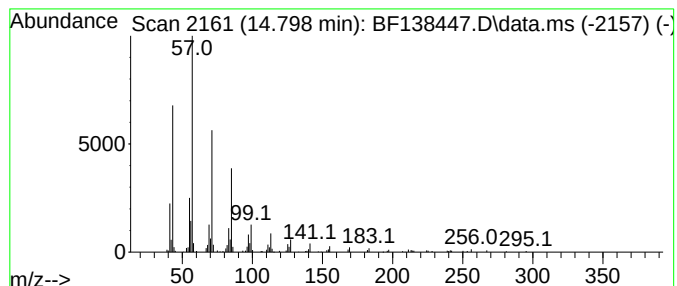
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 11 Heptadecane, 9-octyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.798	5.95 ng	149147	Perylene-d12	15.492

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptacosane	380	C27H56	000593-49-7	91
2			Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
3			Eicosane, 7-hexyl-	366	C26H54	055333-99-8	91
4			Pentacosane	352	C25H52	000629-99-2	91
5			Eicosane	282	C20H42	000112-95-8	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF070324\
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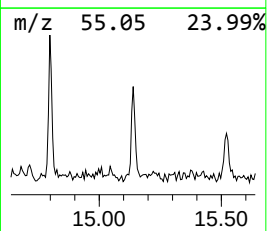
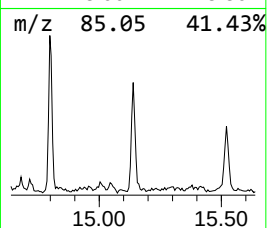
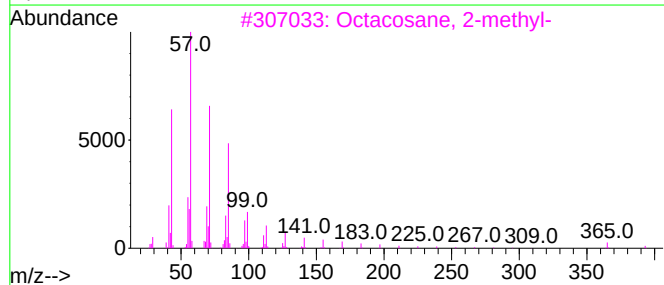
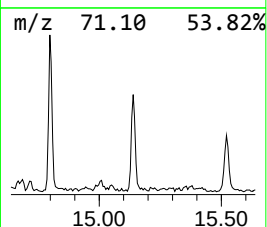
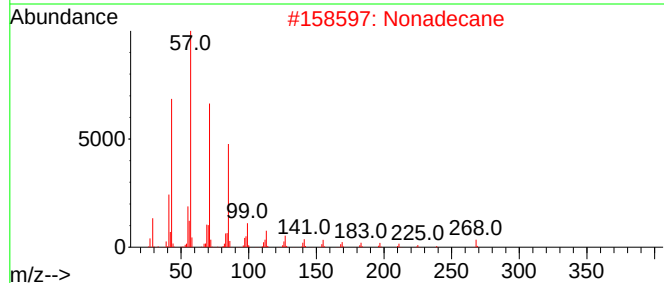
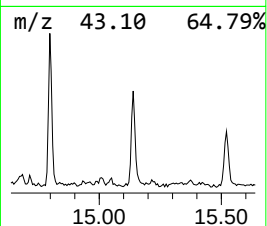
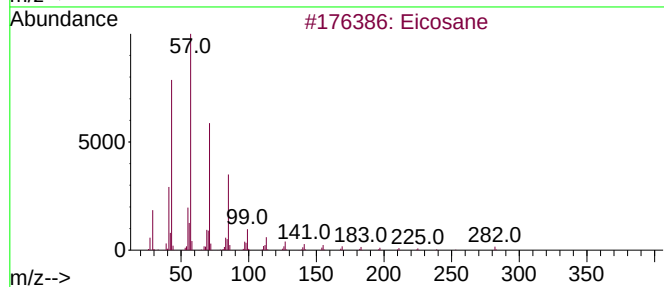
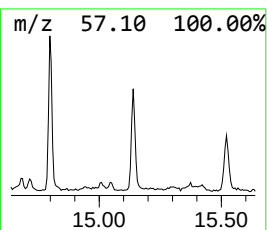
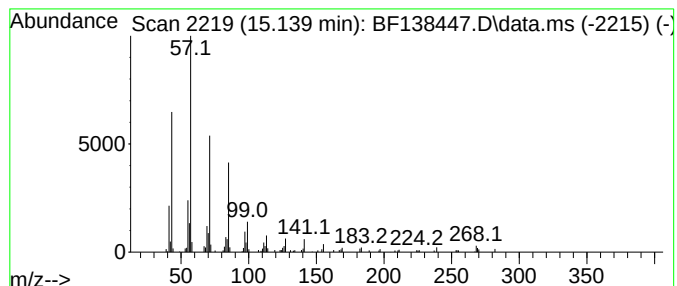
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 12 Eicosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.139	4.82 ng	121017	Perylene-d12	15.492

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Eicosane	282	C20H42	000112-95-8	98
2			Nonadecane	268	C19H40	000629-92-5	96
3			Octacosane, 2-methyl-	408	C29H60	001560-98-1	91
4			Tetratetracontane	619	C44H90	007098-22-8	91
5			Octacosane	394	C28H58	000630-02-4	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF070324\
Data File : BF138447.D
Acq On : 03 Jul 2024 15:42
Operator : CG\JU
Sample : P3141-02
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
B-140-SB01

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062824.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
Butane, 2-metho...	2.187	69.6	ng	3126250	1	6.869	898171	20.0
Propylene Glycol	3.410	3.4	ng	153110	1	6.869	898171	20.0
2-Pentanone, 4-...	5.092	10.2	ng	459514	1	6.869	898171	20.0
1-Phenoxypropan...	8.457	2.7	ng	134558	2	8.151	1013530	20.0
unknown9.998	9.998	2.2	ng	110910	3	9.904	1020880	20.0
n-Hexadecanoic ...	11.916	3.7	ng	151095	4	11.392	821671	20.0
Octacosane	13.545	3.7	ng	118900	5	14.027	646170	20.0
Sulfurous acid,...	13.874	9.5	ng	307086	5	14.027	646170	20.0
Heptacosane	14.186	6.2	ng	199070	5	14.027	646170	20.0
Eicosane, 7-hexyl-	14.492	6.1	ng	197567	5	14.027	646170	20.0
Heptadecane, 9-...	14.798	6.0	ng	149147	6	15.492	501718	20.0
Eicosane	15.139	4.8	ng	121017	6	15.492	501718	20.0