

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091424\
 Data File : BF139358.D
 Acq On : 14 Sep 2024 09:58
 Operator : RC/JU
 Sample : PB163293BL
 Misc :
 ALS Vial : 3 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PB163293BL

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-BF091324.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF139358.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.246	18	26	32	rVB	42008	67318	2.16%	0.357%
2	5.122	509	515	525	rBB	87206	157070	5.04%	0.834%
3	5.504	573	580	586	rBV	1662166	2435626	78.18%	12.934%
4	6.504	743	750	756	rBV	1568775	2504677	80.40%	13.300%
5	6.875	808	813	818	rBB	419481	508794	16.33%	2.702%
6	7.440	902	909	914	rBV	1140932	1635443	52.49%	8.685%
7	8.157	1025	1031	1036	rBV	516098	647700	20.79%	3.439%
8	9.234	1207	1214	1219	rBV	2250605	2969992	95.33%	15.771%
9	9.910	1323	1329	1334	rBV	597920	732700	23.52%	3.891%
10	10.698	1457	1463	1468	rBV	1393242	1829437	58.72%	9.715%
11	11.398	1576	1582	1587	rBV	614494	789050	25.33%	4.190%
12	12.986	1845	1852	1857	rBV	2257324	3115452	100.00%	16.544%
13	14.027	2024	2029	2041	rBV	474194	601390	19.30%	3.194%
14	14.810	2156	2162	2168	rBV	23772	32253	1.04%	0.171%
15	15.151	2215	2220	2227	rVB	32881	46194	1.48%	0.245%
16	15.498	2270	2279	2283	rBV	310572	472276	15.16%	2.508%
17	15.533	2283	2285	2293	rVB	45338	55739	1.79%	0.296%
18	15.974	2353	2360	2371	rVB	37053	64775	2.08%	0.344%
19	16.480	2439	2446	2457	rVB	31457	61587	1.98%	0.327%
20	17.080	2537	2548	2562	rVB2	24630	62247	2.00%	0.331%
21	17.792	2661	2669	2681	rVB3	15088	41838	1.34%	0.222%

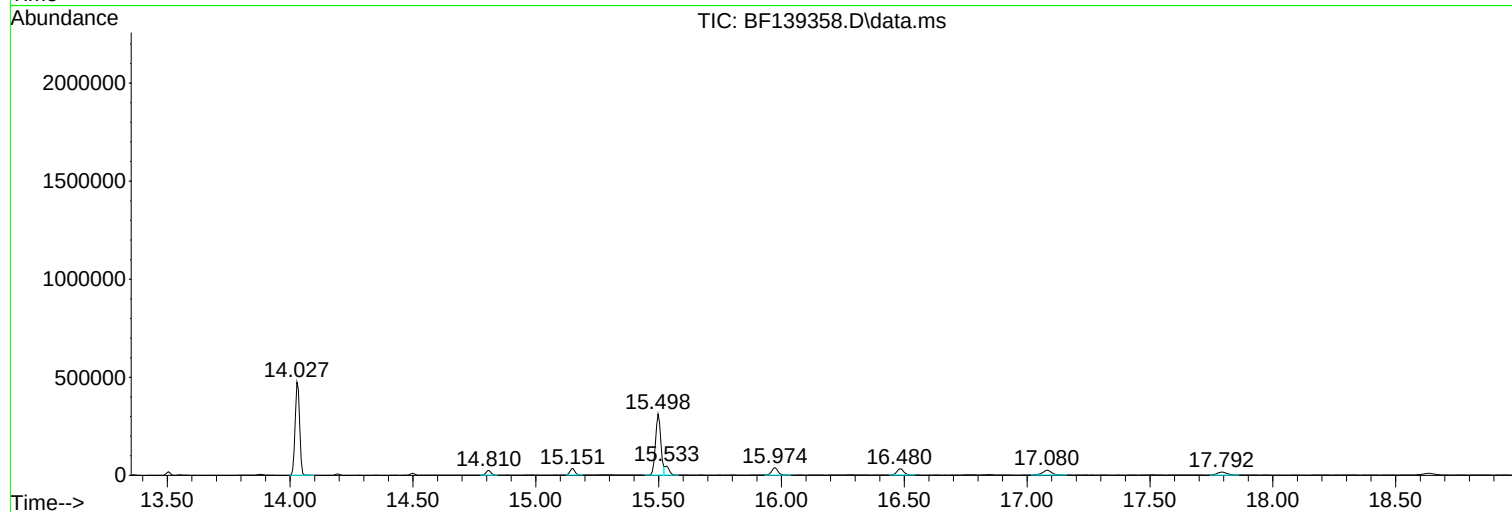
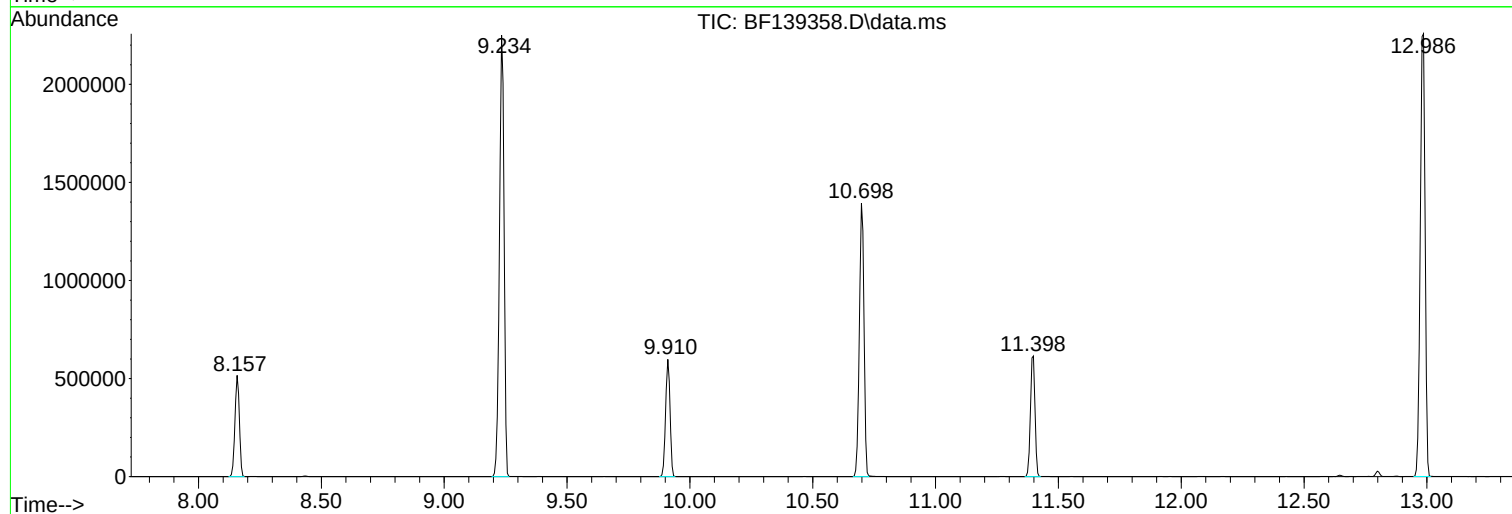
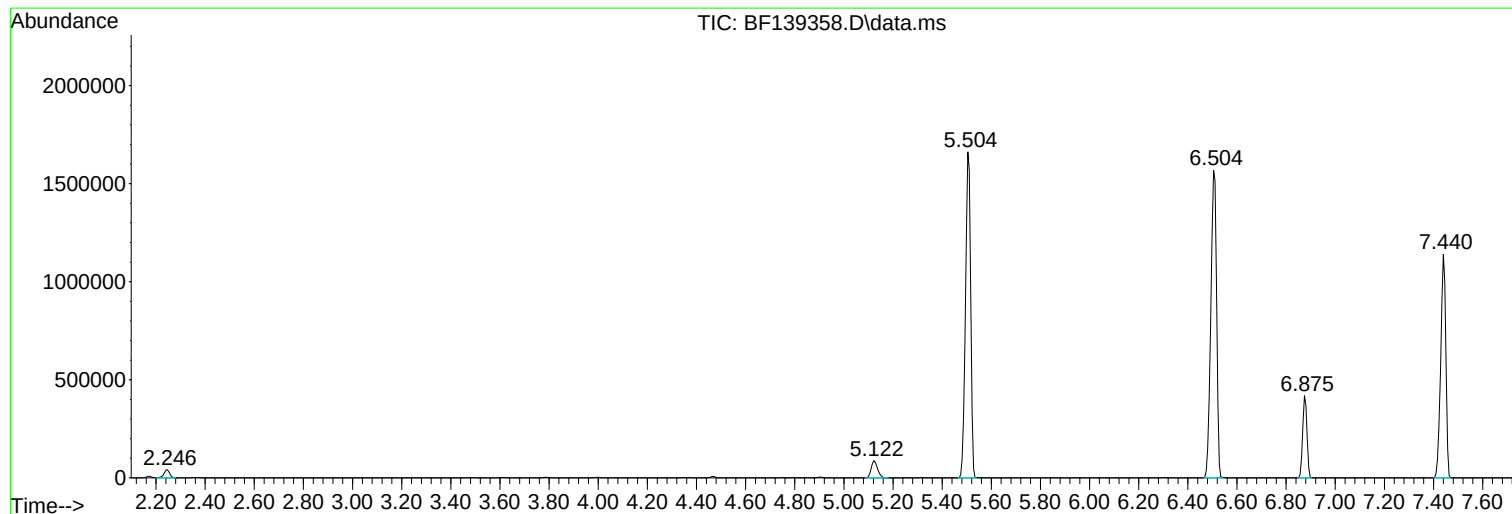
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091324.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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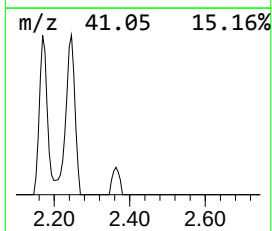
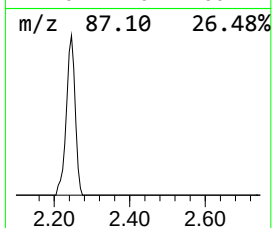
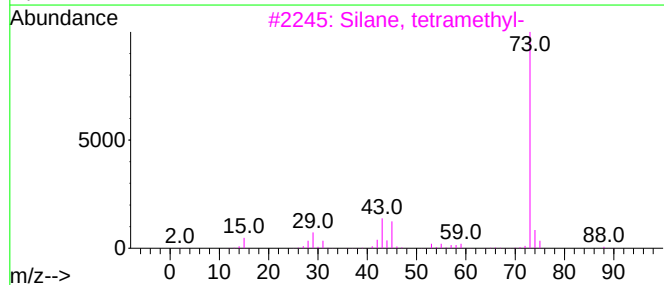
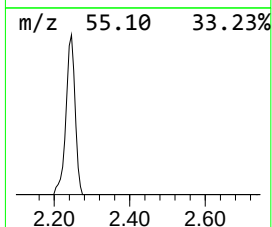
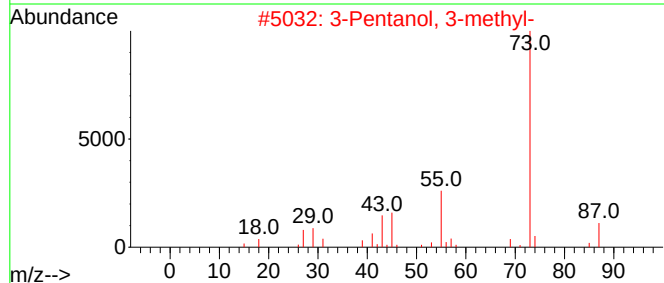
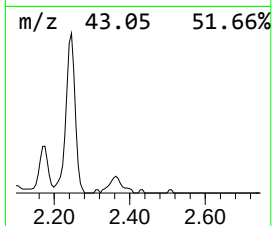
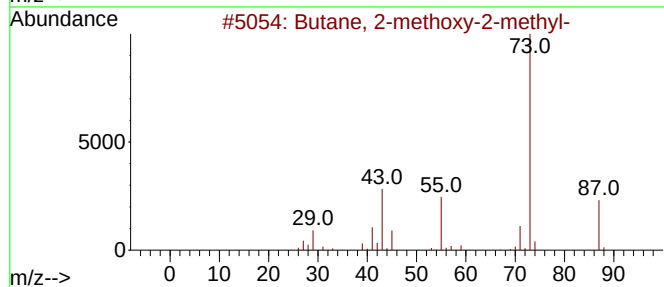
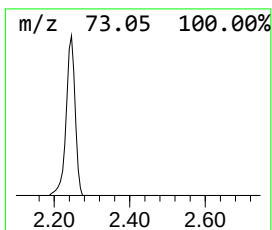
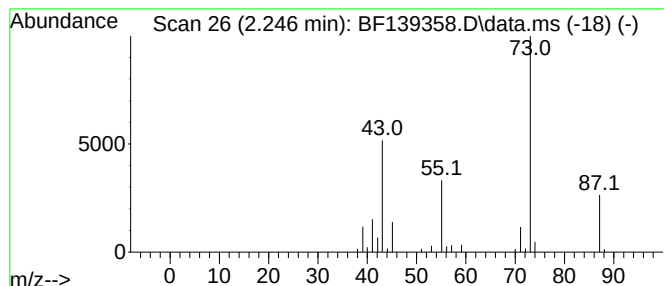
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.246	2.65 ng	67318	1,4-Dichlorobenzene-d4	6.875

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2			3-Pentanol, 3-methyl-	102	C6H14O	000077-74-7	37
3			Silane, tetramethyl-	88	C4H12Si	000075-76-3	35
4			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	33
5			2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	28



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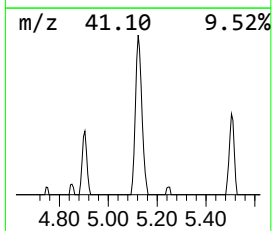
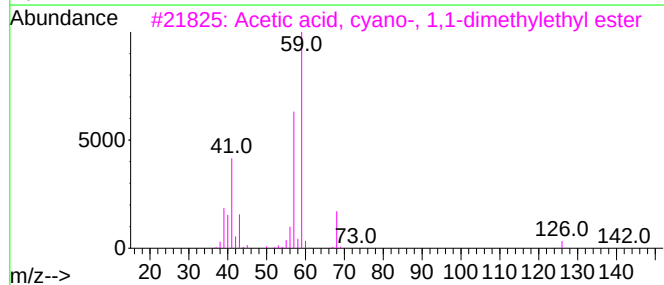
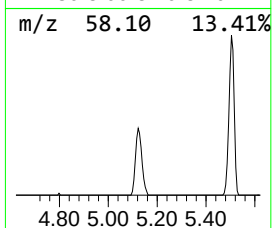
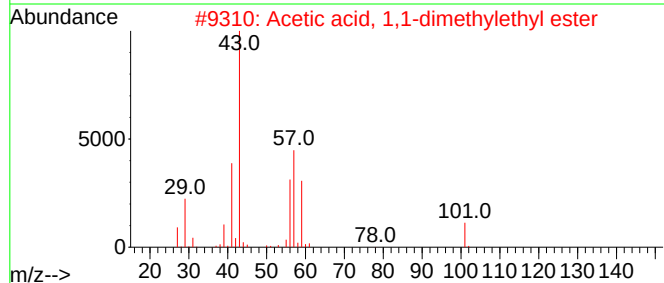
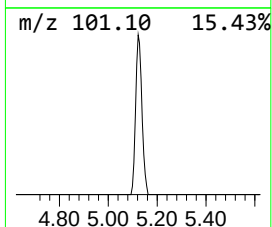
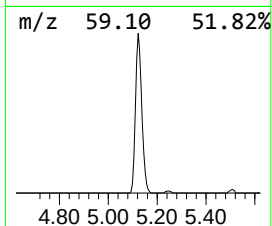
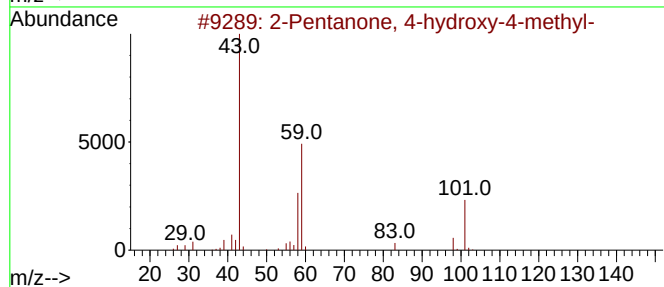
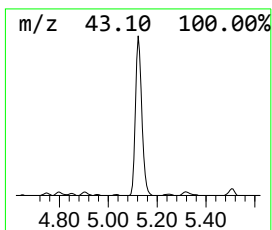
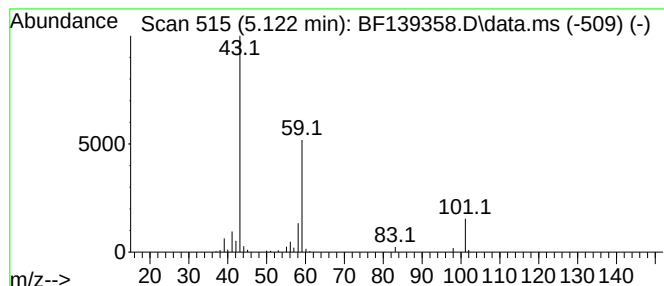
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091324.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.122	6.17 ng	157070	1,4-Dichlorobenzene-d4	6.875

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56		
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	28		
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25		
4	Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	23		
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16		



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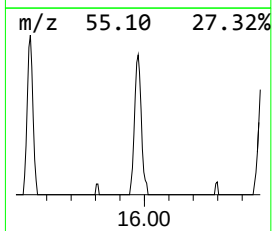
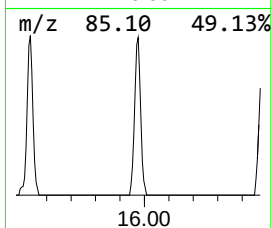
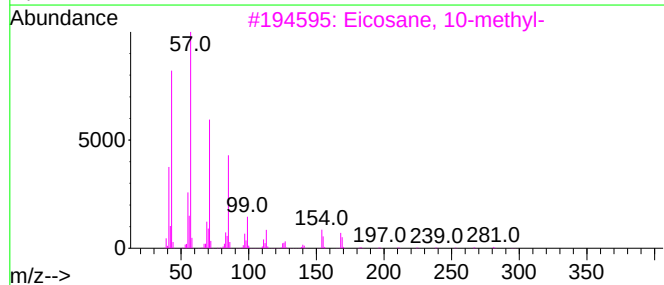
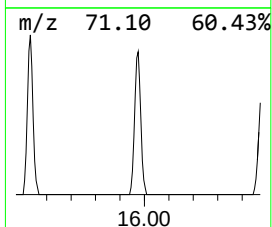
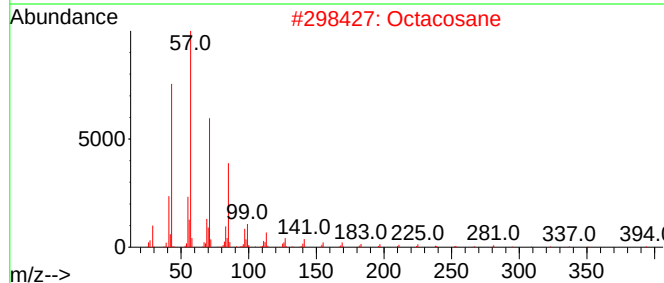
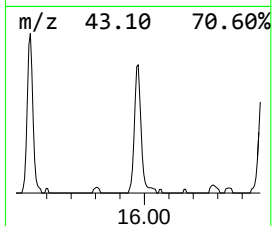
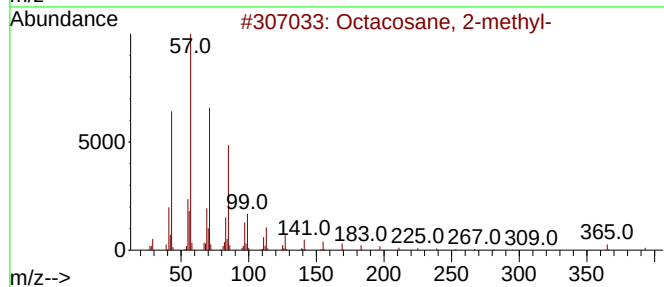
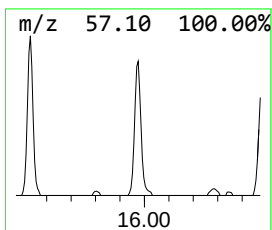
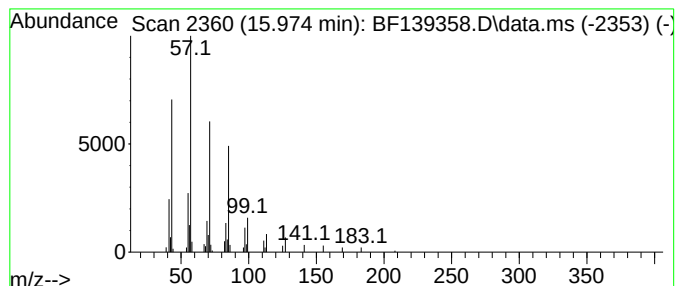
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Octacosane, 2-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.974	2.74 ng	64775	Perylene-d12	15.498

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octacosane, 2-methyl-	408	C29H60	001560-98-1	91
2			Octacosane	394	C28H58	000630-02-4	91
3			Eicosane, 10-methyl-	296	C21H44	054833-23-7	90
4			Tetracosane	338	C24H50	000646-31-1	86
5			Octadecane	254	C18H38	000593-45-3	86



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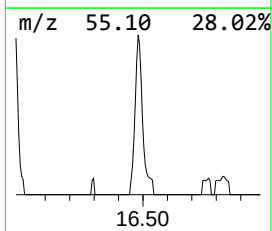
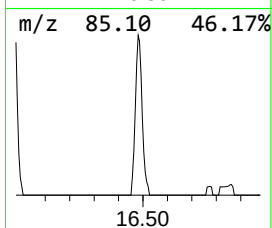
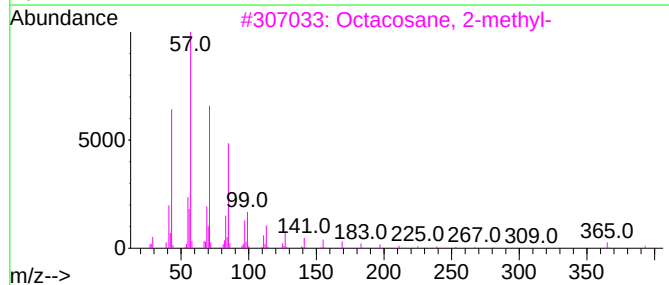
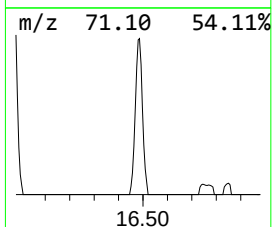
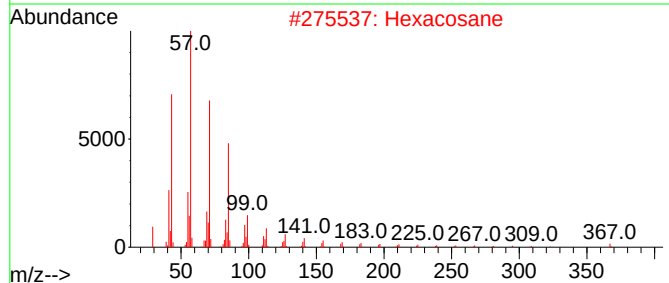
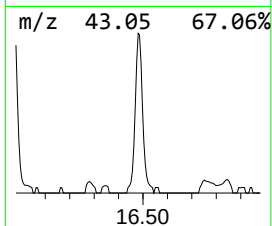
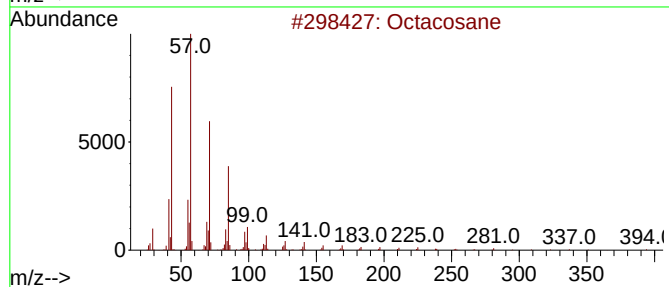
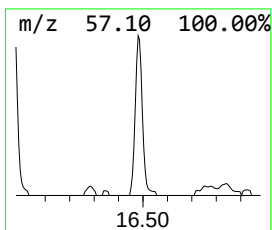
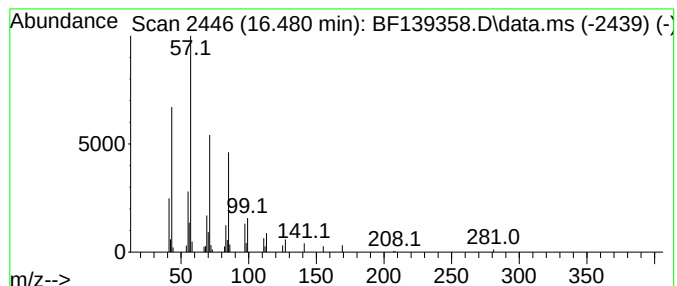
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Octacosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.480	2.61 ng	61587	Perylene-d12	15.498

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Octacosane	394	C28H58	000630-02-4	91
2		Hexacosane	366	C26H54	000630-01-3	91
3		Octacosane, 2-methyl-	408	C29H60	001560-98-1	91
4		Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
5		Tetratetracontane	619	C44H90	007098-22-8	91



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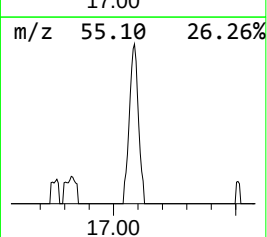
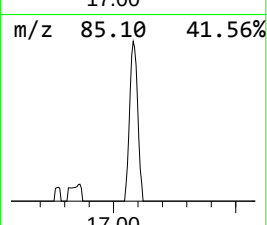
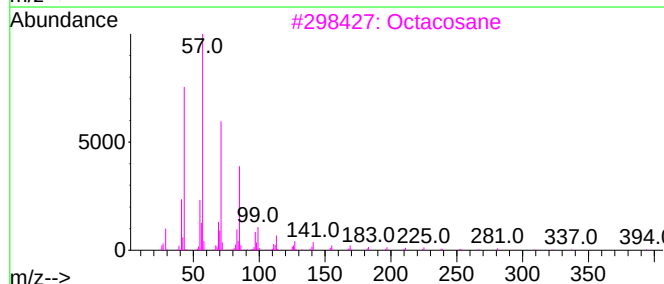
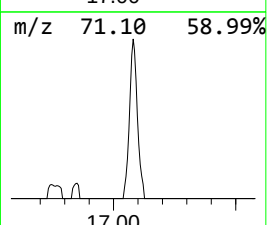
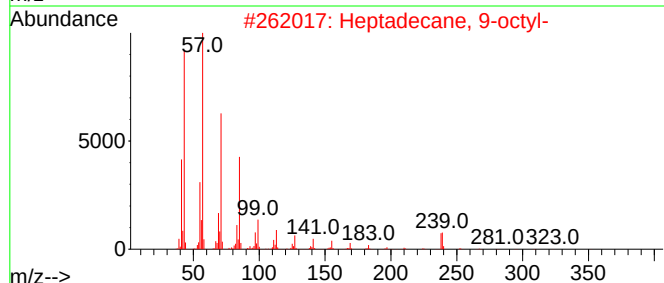
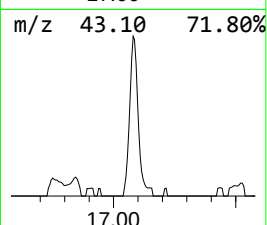
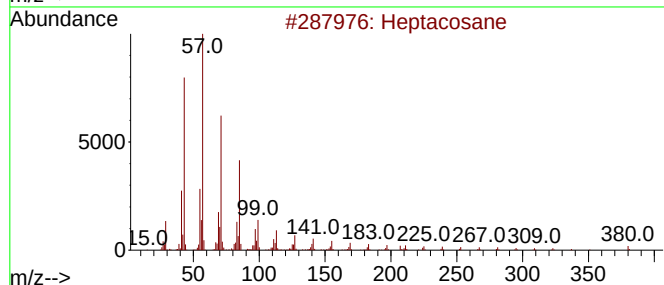
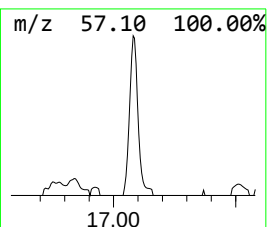
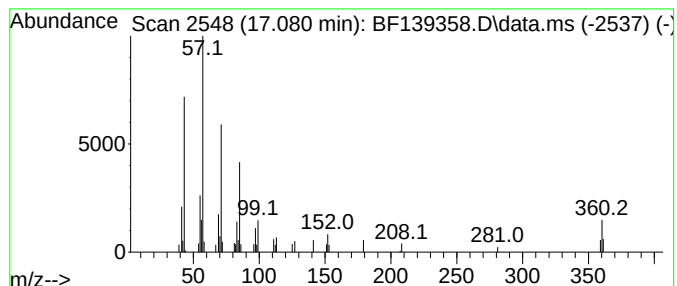
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 Heptacosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.080	2.64 ng	62247	Perylene-d12	15.498

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptacosane	380	C27H56	000593-49-7	74
2			Heptadecane, 9-octyl-	352	C25H52	007225-64-1	74
3			Octacosane	394	C28H58	000630-02-4	74
4			Tetratetracontane	619	C44H90	007098-22-8	74
5			Tetracosane, 11-decyl-	479	C34H70	055429-84-0	74



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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	2.246	2.6	ng	67318	1	6.875	508794	20.0
2-Pentanone, 4-...	5.122	6.2	ng	157070	1	6.875	508794	20.0
Octacosane, 2-m...	15.974	2.7	ng	64775	6	15.498	472276	20.0
Octacosane	16.480	2.6	ng	61587	6	15.498	472276	20.0
Heptacosane	17.080	2.6	ng	62247	6	15.498	472276	20.0