

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF020222\
 Data File : BF126786.D
 Acq On : 02 Feb 2022 15:16
 Operator : CG/JU
 Sample : PB142123BL
 Misc :
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PB142123BL

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-BF020222.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF126786.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.358	35	46	52	rVB	129640	189108	3.62%	0.572%
2	5.581	588	594	597	rBV	3839584	4469469	85.62%	13.510%
3	6.569	755	762	765	rBV	3799299	4619255	88.49%	13.963%
4	6.946	822	826	830	rBB	1081358	888308	17.02%	2.685%
5	7.510	916	922	925	rBV	2561863	3001646	57.50%	9.073%
6	8.228	1039	1044	1048	rBV	1243994	1170961	22.43%	3.540%
7	9.310	1221	1228	1231	rBV	4507702	4693647	89.91%	14.188%
8	9.987	1338	1343	1347	rBV	1470609	1276771	24.46%	3.859%
9	10.781	1472	1478	1481	rBV	3253055	3177159	60.86%	9.604%
10	11.481	1593	1597	1600	rBV	1687799	1391229	26.65%	4.205%
11	13.075	1863	1868	1871	rBV	5317560	5220099	100.00%	15.779%
12	14.127	2043	2047	2050	rBV	1296416	1117804	21.41%	3.379%
13	14.904	2175	2179	2183	rVB	89549	85272	1.63%	0.258%
14	15.263	2235	2240	2245	rVB	112580	130145	2.49%	0.393%
15	15.639	2298	2304	2318	rBV2	541301	893750	17.12%	2.702%
16	16.127	2381	2387	2393	rBV	117862	163208	3.13%	0.493%
17	16.668	2471	2479	2491	rBV	94499	190603	3.65%	0.576%
18	17.298	2578	2586	2593	rBV2	76700	165829	3.18%	0.501%
19	18.057	2706	2715	2723	rBV2	60507	150999	2.89%	0.456%
20	18.951	2856	2867	2870	rBV5	35050	87354	1.67%	0.264%

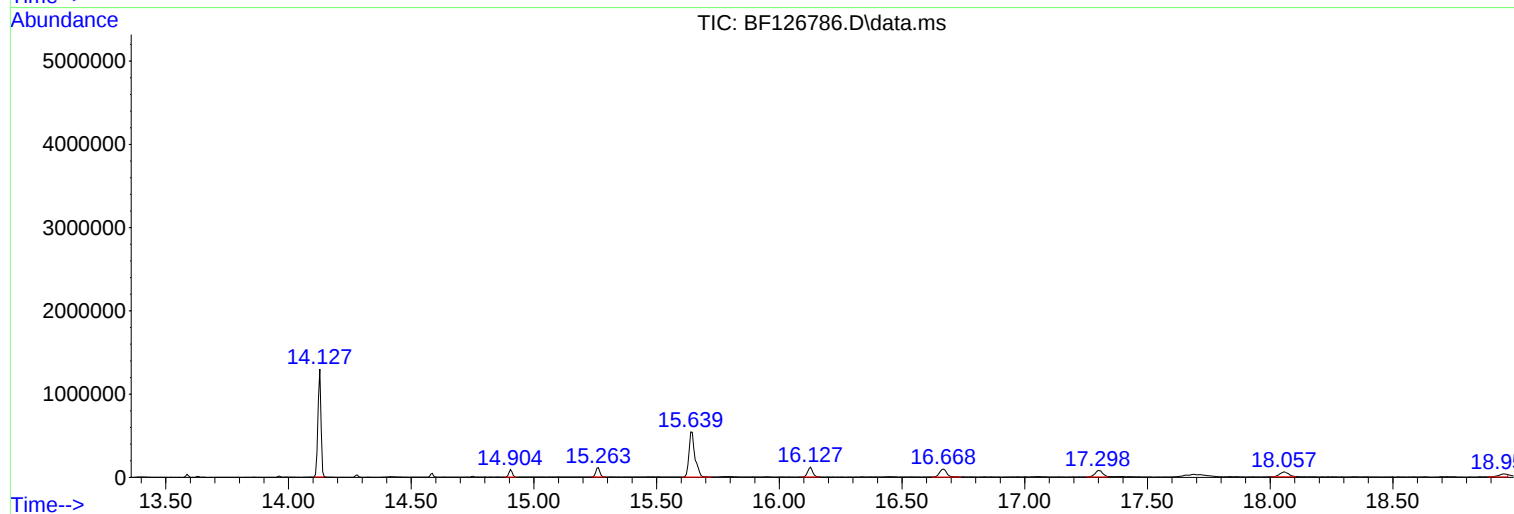
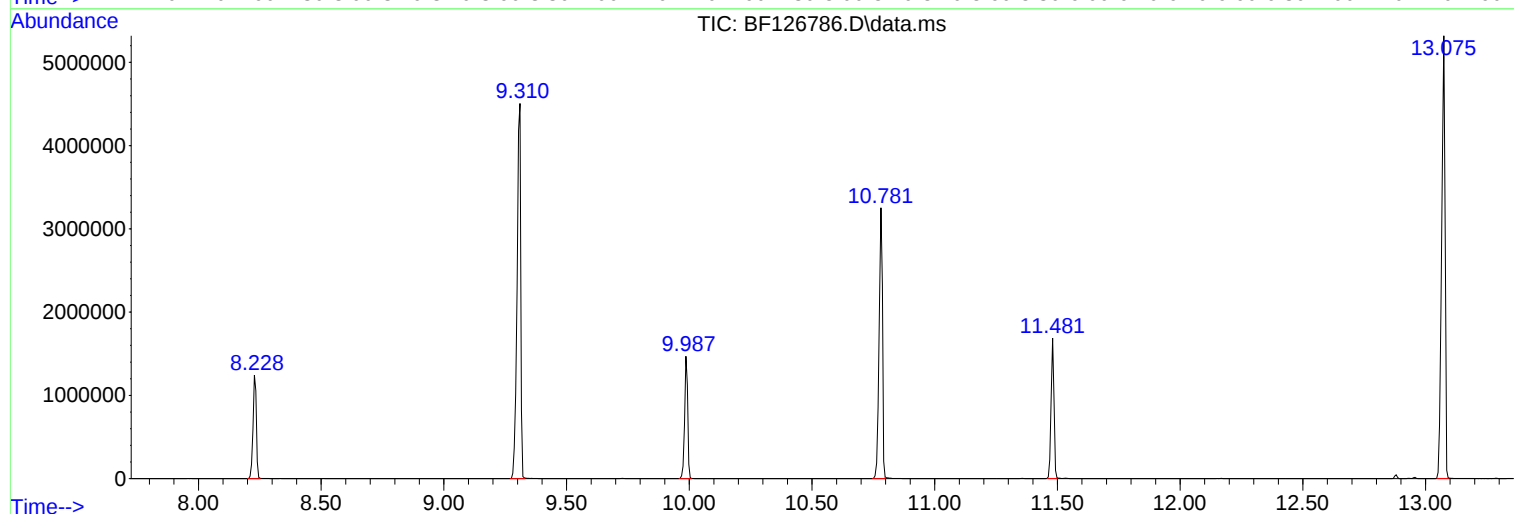
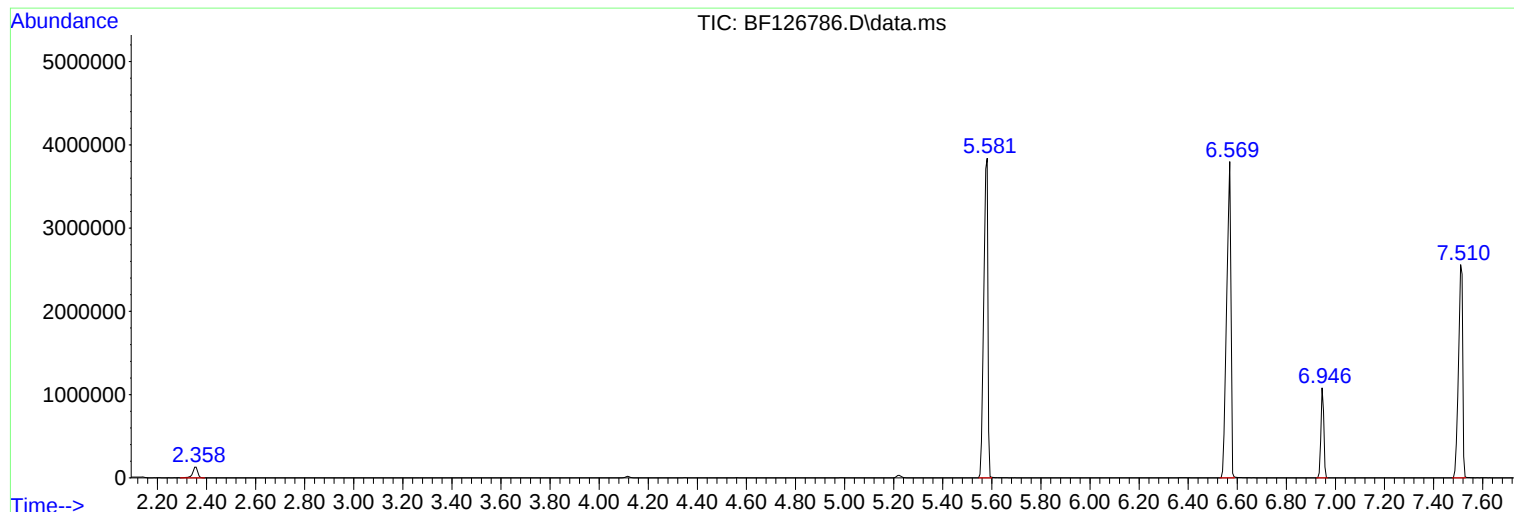
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF020222.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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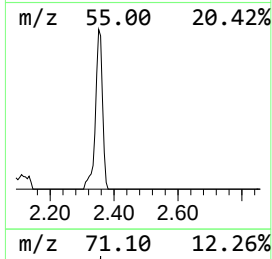
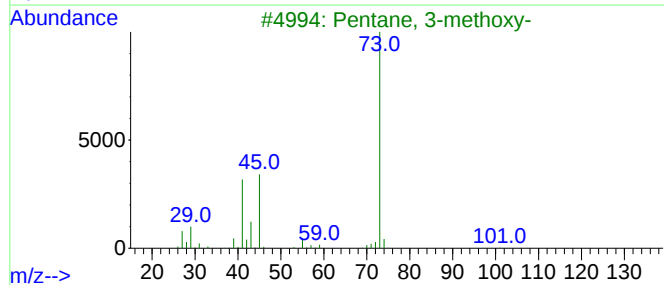
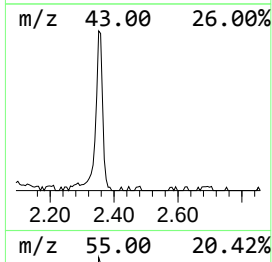
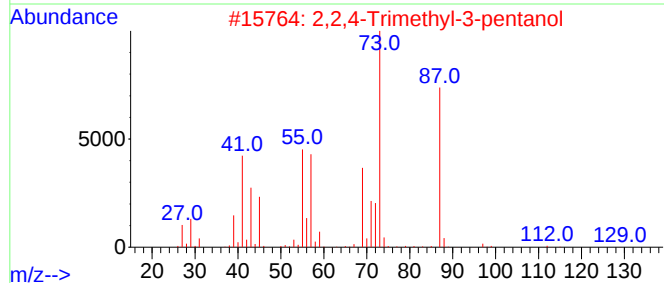
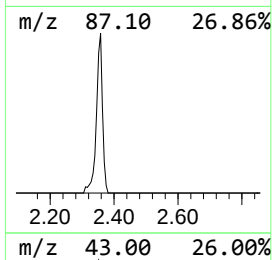
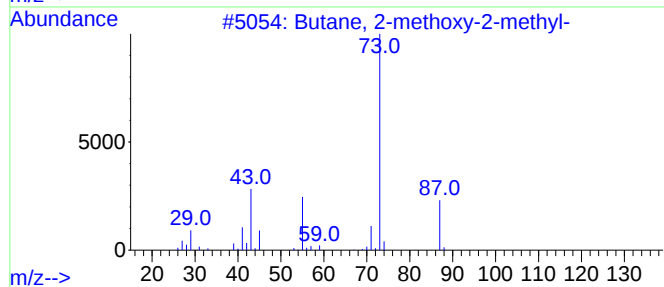
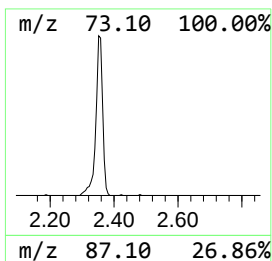
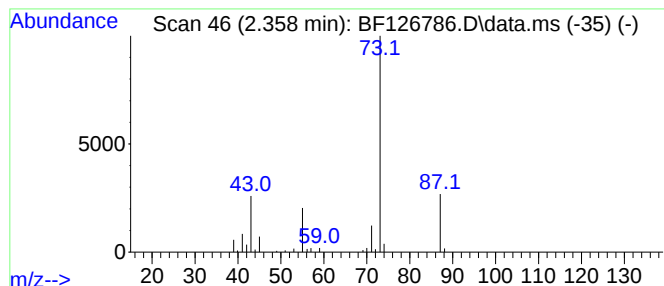
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST0.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.
2.358	4.26 ng	189108	1,4-Dichlorobenzene-d4	6.946

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17
4			3-Hexanol, 2-methyl-	116	C7H16O	000617-29-8	17
5			N-Ethylformamide	73	C3H7NO	000627-45-2	9



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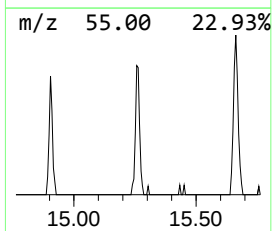
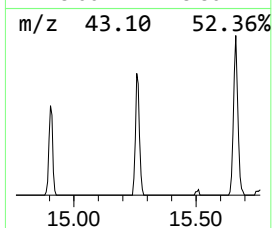
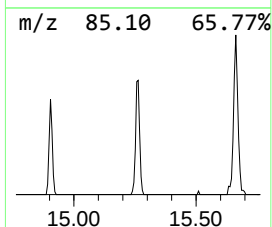
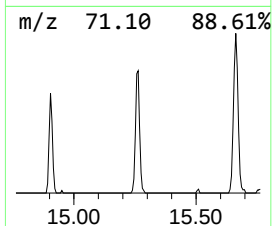
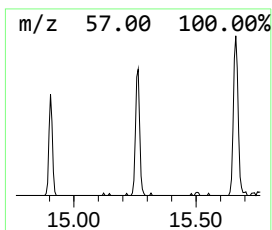
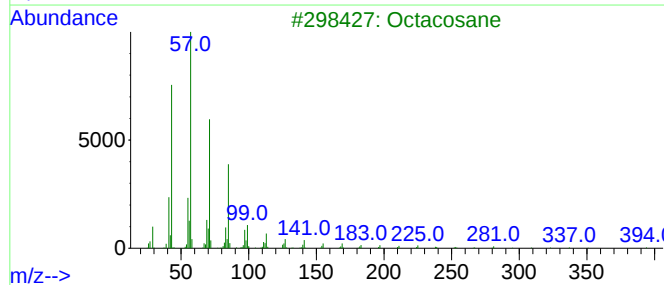
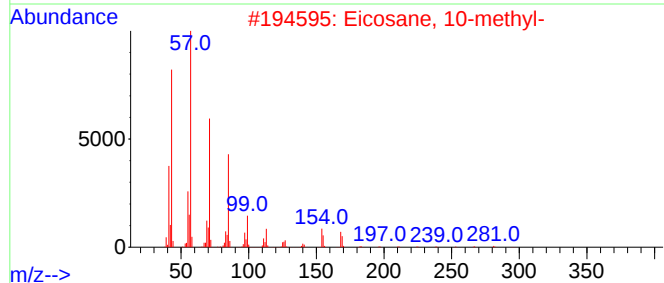
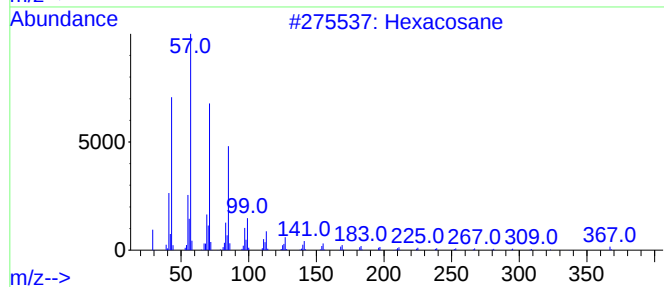
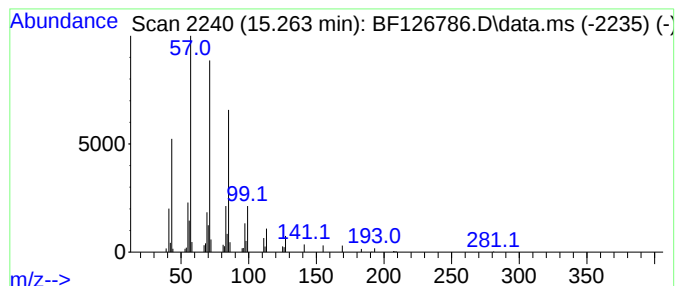
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF020222.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 Octacosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.263	2.91 ng	130145	Perylene-d12	15.639

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Hexacosane	366	C26H54	000630-01-3	86
2		Eicosane, 10-methyl-	296	C21H44	054833-23-7	80
3		Octacosane	394	C28H58	000630-02-4	72
4		Sulfurous acid, butyl decyl ester	278	C14H30O3S	1000309-17-7	64
5		Sulfurous acid, decyl 2-propyl e...	264	C13H28O3S	1000309-12-1	64



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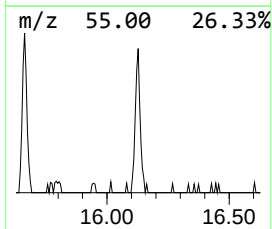
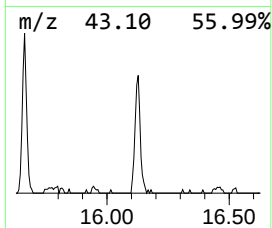
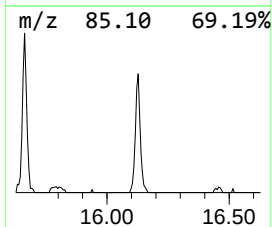
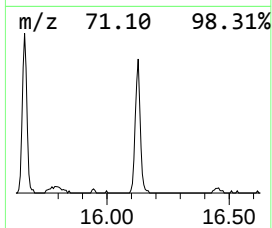
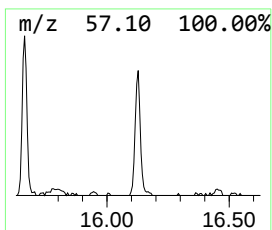
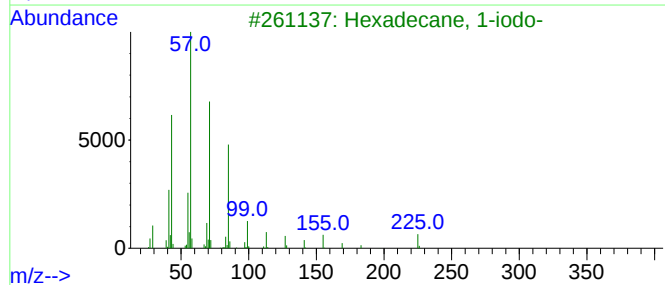
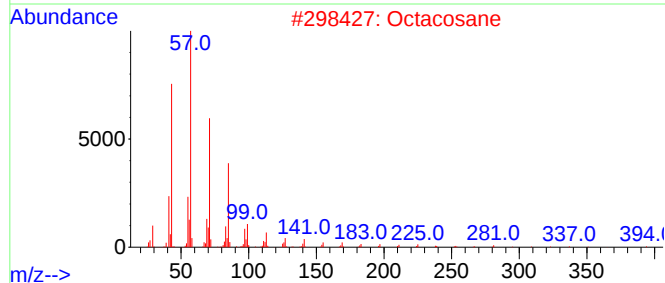
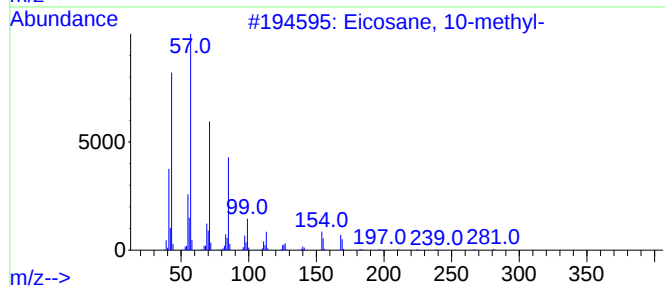
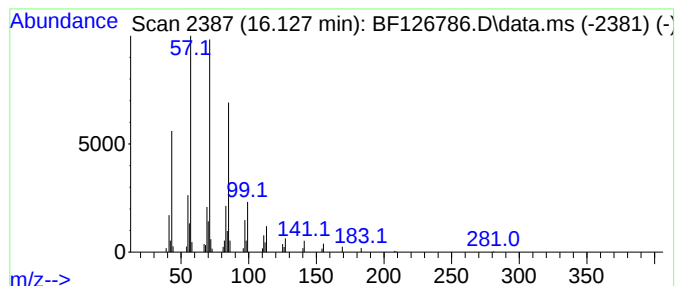
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Eicosane, 10-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.127	3.65 ng	163208	Perylene-d12	15.639

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Eicosane, 10-methyl-	296	C21H44	054833-23-7	86
2			Octacosane	394	C28H58	000630-02-4	72
3			Hexadecane, 1-iodo-	352	C16H33I	000544-77-4	72
4			Nonadecane	268	C19H40	000629-92-5	72
5			Heneicosane	296	C21H44	000629-94-7	68



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Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB142123BL

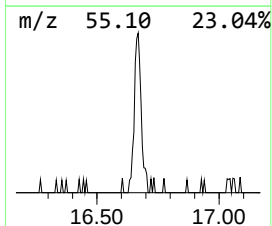
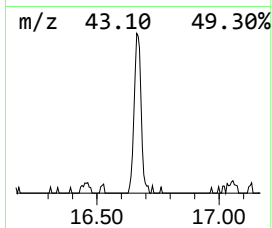
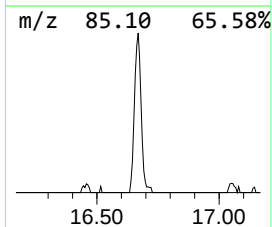
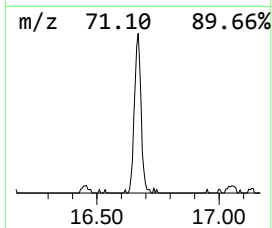
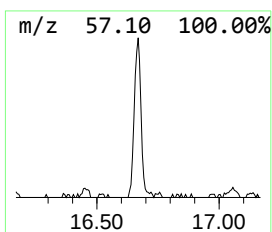
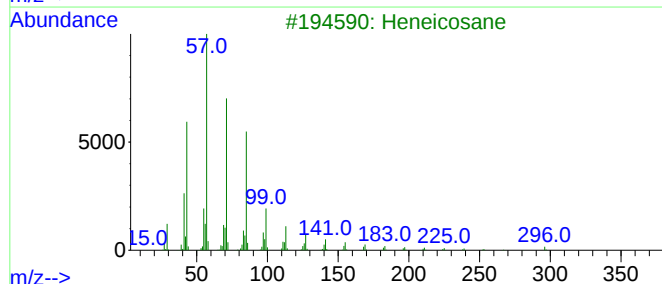
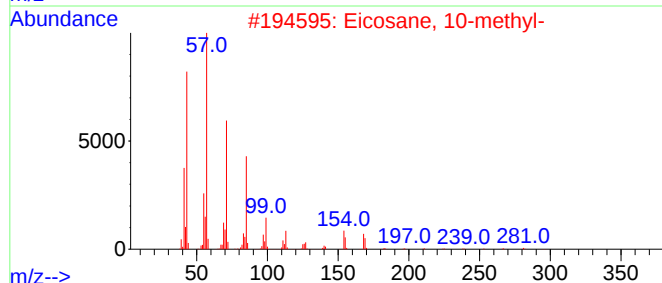
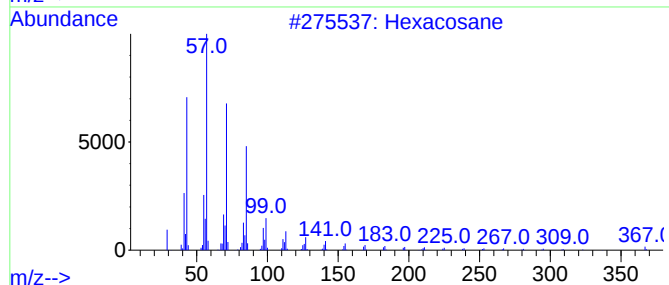
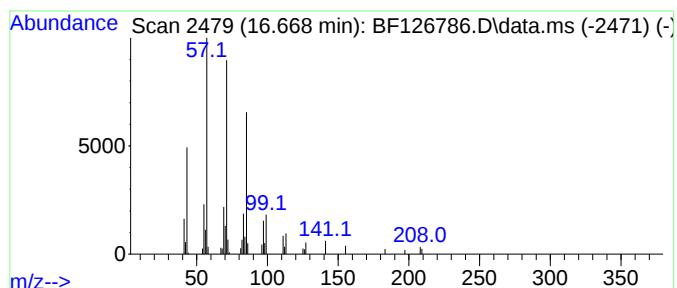
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 Heneicosane Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.668	4.27 ng	190603	Perylene-d12	15.639

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexacosane	366	C26H54	000630-01-3	87
2			Eicosane, 10-methyl-	296	C21H44	054833-23-7	86
3			Heneicosane	296	C21H44	000629-94-7	86
4			9-Methylheneicosane	310	C22H46	070475-51-3	86
5			Octadecane	254	C18H38	000593-45-3	86



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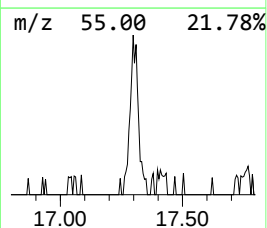
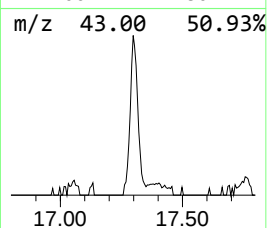
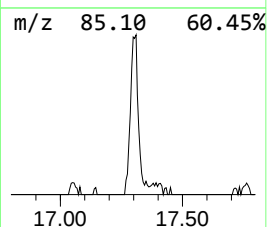
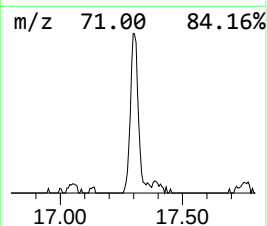
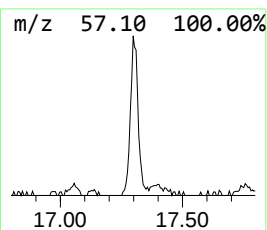
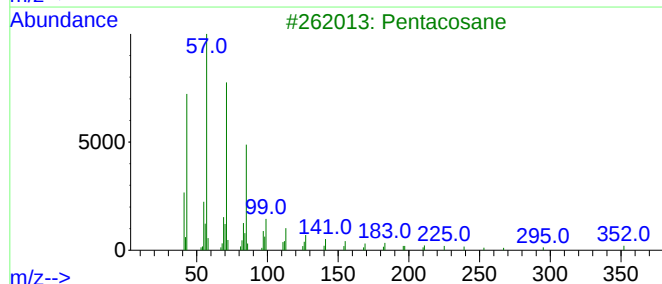
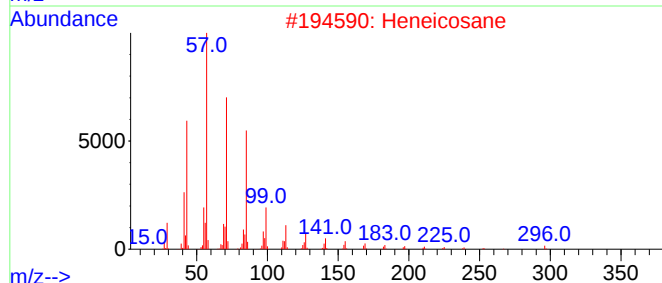
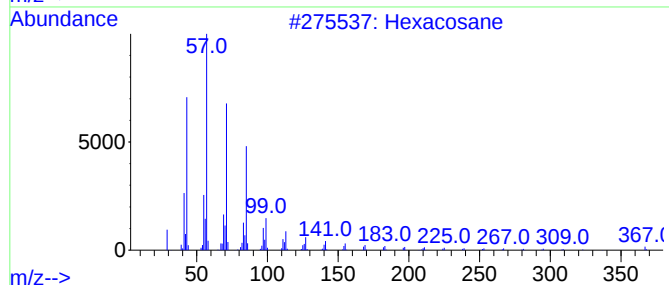
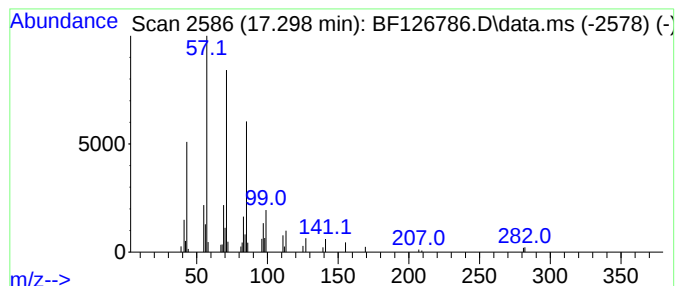
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 Hexacosane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.298	3.71 ng	165829	Perylene-d12	15.639

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexacosane	366	C26H54	000630-01-3	91
2			Heneicosane	296	C21H44	000629-94-7	91
3			Pentacosane	352	C25H52	000629-99-2	91
4			Octacosane, 2-methyl-	408	C29H60	001560-98-1	91
5			Heptadecane	240	C17H36	000629-78-7	91



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PB142123BL

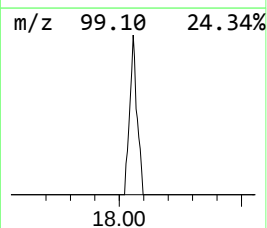
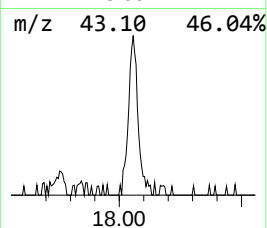
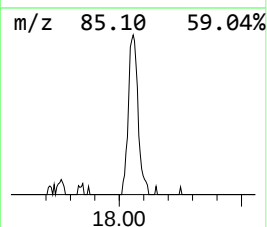
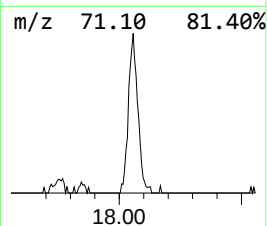
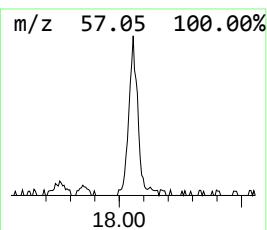
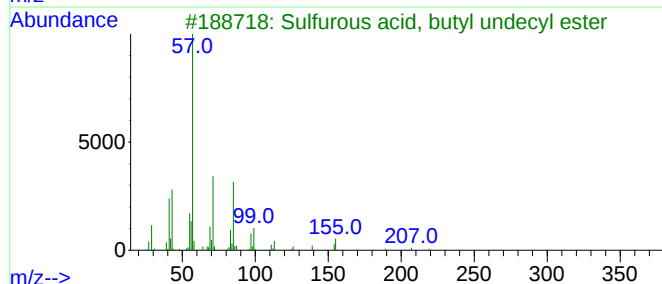
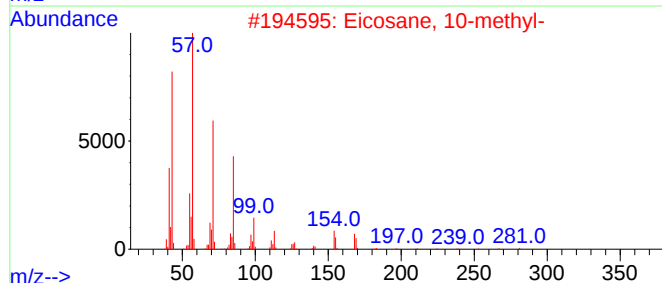
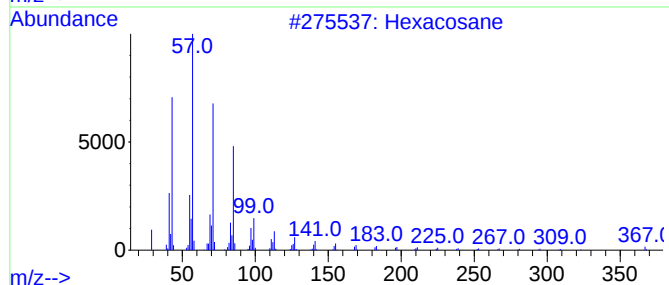
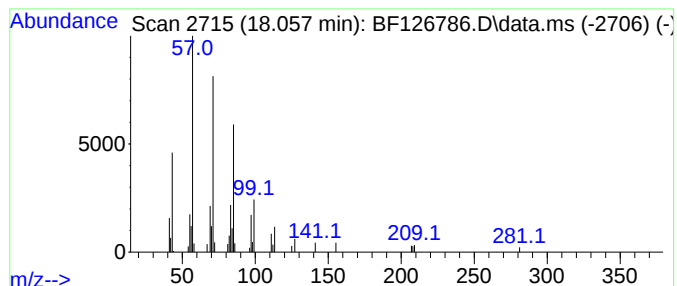
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF020222.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Sulfurous acid, butyl undec... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.057	3.38 ng	150999	Perylene-d12	15.639

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexacosane	366	C26H54	000630-01-3	83
2			Eicosane, 10-methyl-	296	C21H44	054833-23-7	80
3			Sulfurous acid, butyl undecyl ester	292	C15H32O3S	1000309-17-8	80
4			Sulfurous acid, butyl tridecyl e...	320	C17H36O3S	1000309-18-0	72
5			Tritetracontane	605	C43H88	007098-21-7	72



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF020222\
Data File : BF126786.D
Acq On : 02 Feb 2022 15:16
Operator : CG/JU
Sample : PB142123BL
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB142123BL

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF020222.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...	2.358	4.3	ng	189108	1	6.946	888308	20.0
Octacosane	15.263	2.9	ng	130145	6	15.639	893750	20.0
Eicosane, 10-me...	16.127	3.6	ng	163208	6	15.639	893750	20.0
Heneicosane	16.668	4.3	ng	190603	6	15.639	893750	20.0
Hexacosane	17.298	3.7	ng	165829	6	15.639	893750	20.0
Sulfurous acid,...	18.057	3.4	ng	150999	6	15.639	893750	20.0