

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM083024\
 Data File : BM047406.D
 Acq On : 30 Aug 2024 15:00
 Operator : RC/JU
 Sample : P3794-01
 Misc :
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 CHRT-24376

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_M\Methods\8270-BM082624.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM047406.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.263	61	64	70	rBV	56650	83096	1.08%	0.174%
2	4.557	276	284	290	rBV	165465	234742	3.06%	0.492%
3	5.010	352	361	381	rBV	2570132	3922294	51.12%	8.223%
4	6.569	619	626	650	rBV	2309816	3961420	51.63%	8.305%
5	7.345	750	758	768	rBV	800170	1259771	16.42%	2.641%
6	8.492	946	953	975	rBV	1541506	2718903	35.44%	5.700%
7	10.098	1218	1226	1239	rBV	942433	1621298	21.13%	3.399%
8	10.875	1349	1358	1367	rBV	66720	157267	2.05%	0.330%
9	12.610	1646	1653	1672	rBV	4040797	6317654	82.34%	13.245%
10	13.816	1853	1858	1864	rVB4	56350	116270	1.52%	0.244%
11	13.910	1870	1874	1880	rBV6	31060	77028	1.00%	0.161%
12	14.010	1885	1891	1900	rVV	1411382	2245759	29.27%	4.708%
13	14.239	1926	1930	1931	rBV2	84139	100638	1.31%	0.211%
14	14.263	1931	1934	1939	rVB2	161318	227257	2.96%	0.476%
15	14.798	2021	2025	2030	rBV2	72102	97858	1.28%	0.205%
16	15.304	2106	2111	2116	rBV2	94711	164202	2.14%	0.344%
17	15.398	2122	2127	2132	rVB	214873	312505	4.07%	0.655%
18	15.521	2142	2148	2158	rBV	2946036	4608288	60.06%	9.662%
19	15.786	2186	2193	2197	rBV	305461	524077	6.83%	1.099%
20	16.127	2248	2251	2255	rVB3	197640	223726	2.92%	0.469%
21	16.610	2329	2333	2340	rVB	564201	857965	11.18%	1.799%
22	16.774	2356	2361	2371	rBV	1557547	2426373	31.62%	5.087%
23	17.710	2517	2520	2528	rVB	933139	1200169	15.64%	2.516%
24	19.009	2738	2741	2744	rBV	424809	492618	6.42%	1.033%
25	19.439	2809	2814	2827	rVB	5951269	7672685	100.00%	16.086%
26	20.127	2928	2931	2934	rVV	99039	110963	1.45%	0.233%
27	20.162	2934	2937	2947	rVB	261841	345489	4.50%	0.724%
28	20.745	3033	3036	3043	rVB	353392	491005	6.40%	1.029%
29	21.021	3078	3083	3089	rBV	1589536	2183452	28.46%	4.578%
30	21.156	3103	3106	3109	rVB	227670	250639	3.27%	0.525%
31	23.721	3536	3542	3557	rVB	994608	2692027	35.09%	5.644%

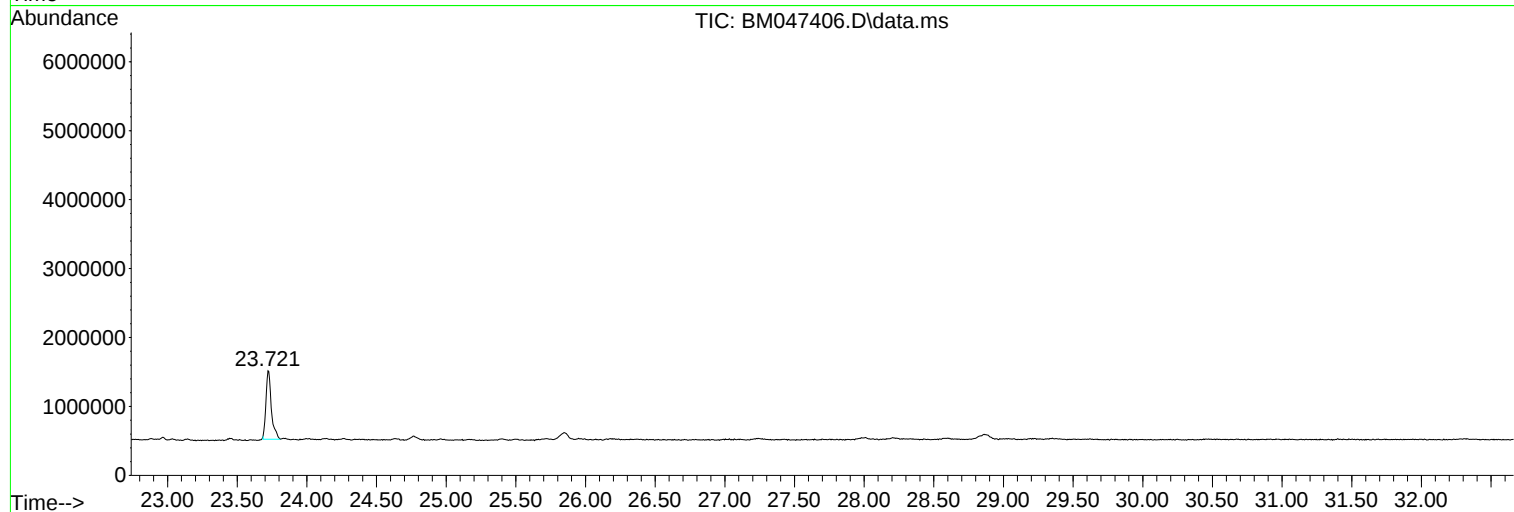
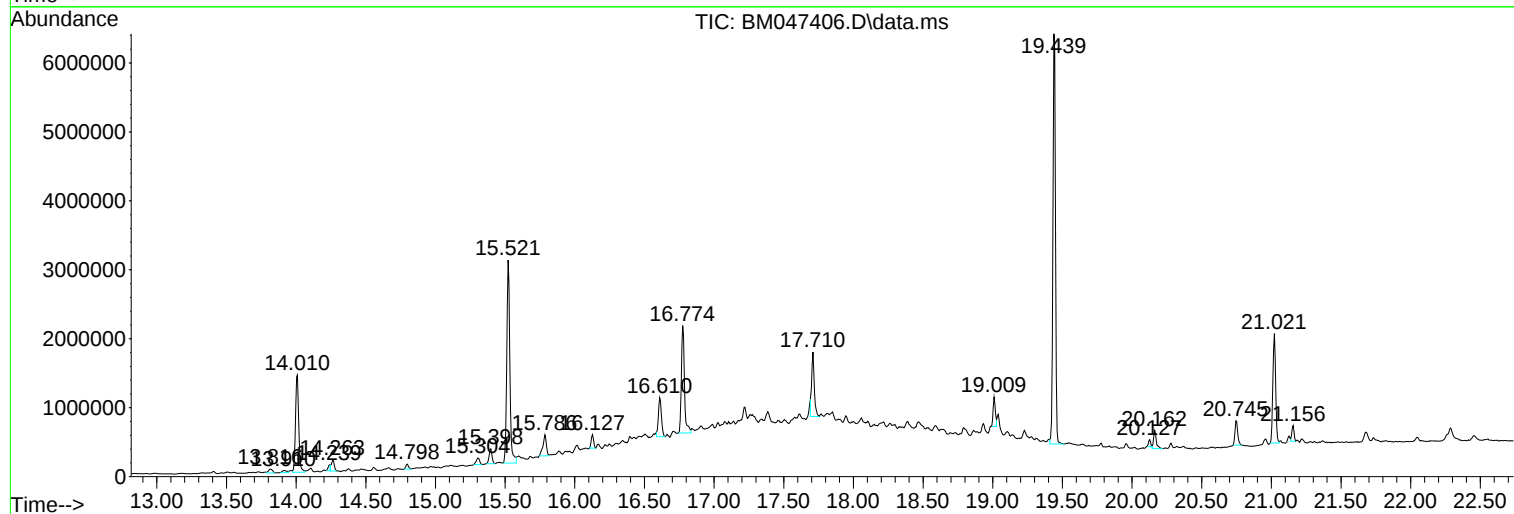
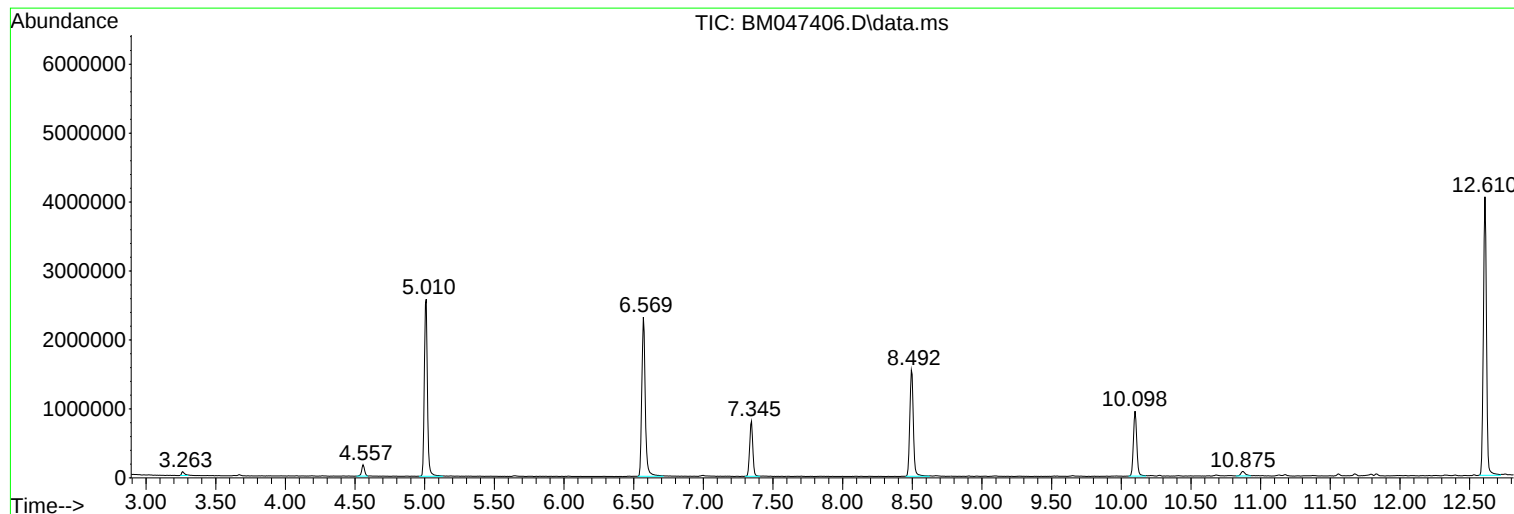
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM082624.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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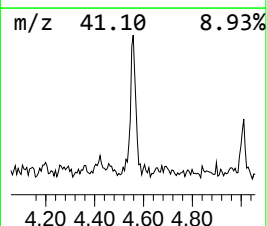
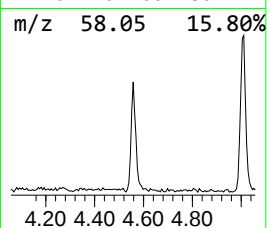
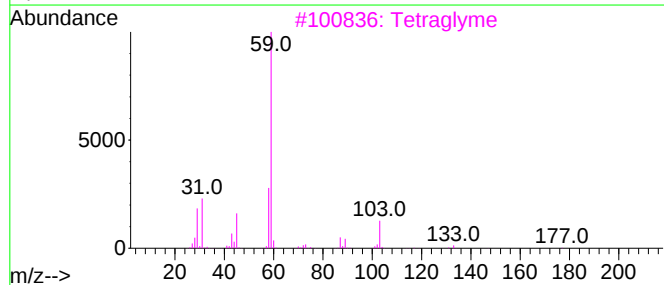
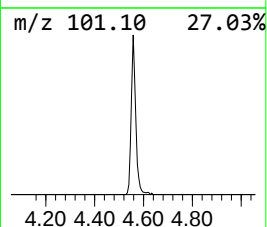
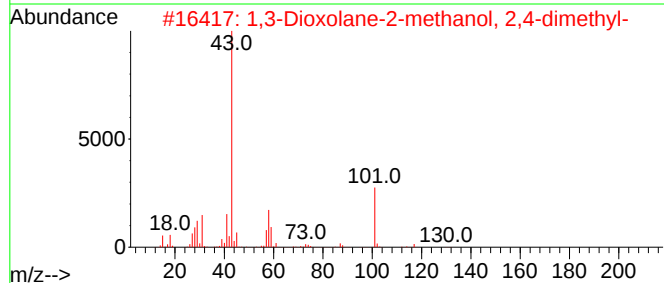
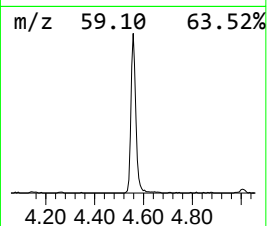
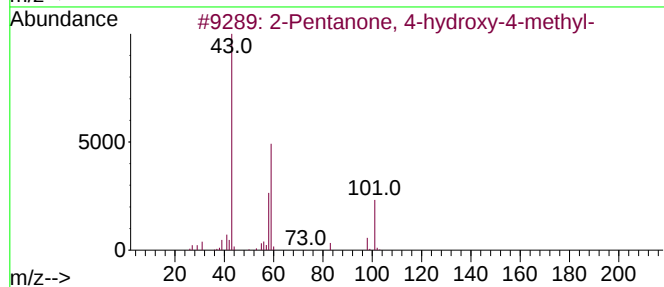
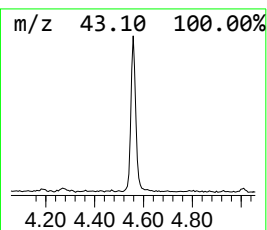
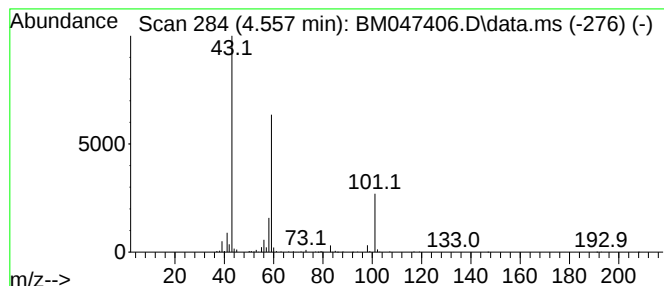
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Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.557	3.73 ng	234742	1,4-Dichlorobenzene-d4	7.345

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64		
2	1,3-Dioxolane-2-methanol, 2,4-di...	132	C6H12O3	053951-43-2	28		
3	Tetraglyme	222	C10H22O5	000143-24-8	25		
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25		
5	4-Hydroxy-3-hexanone	116	C6H12O2	004984-85-4	25		



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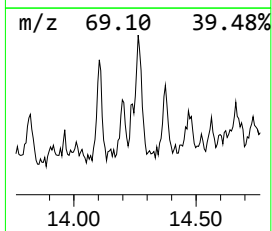
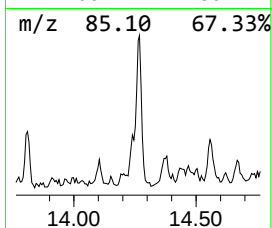
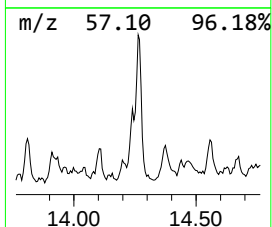
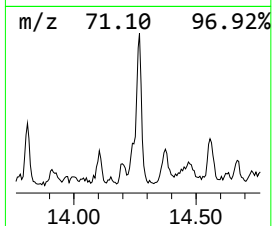
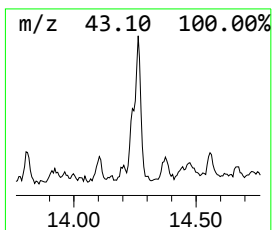
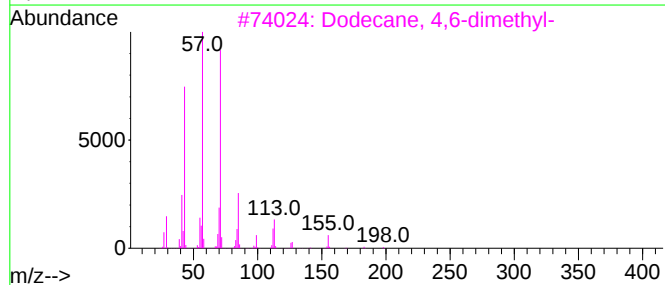
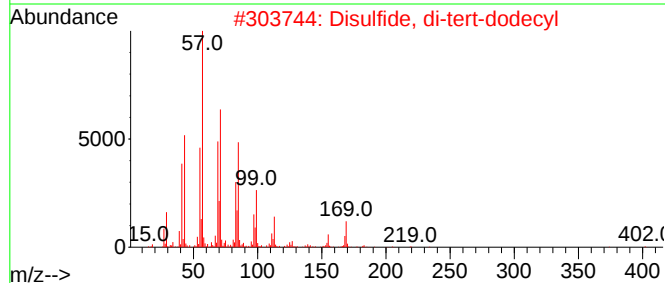
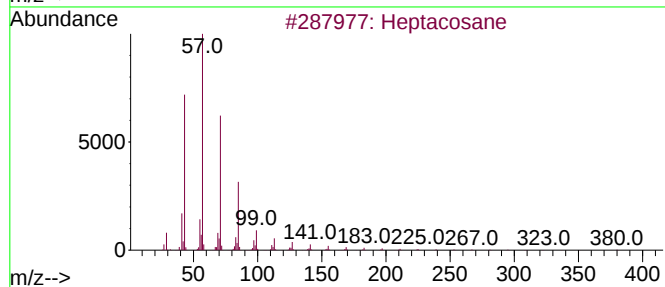
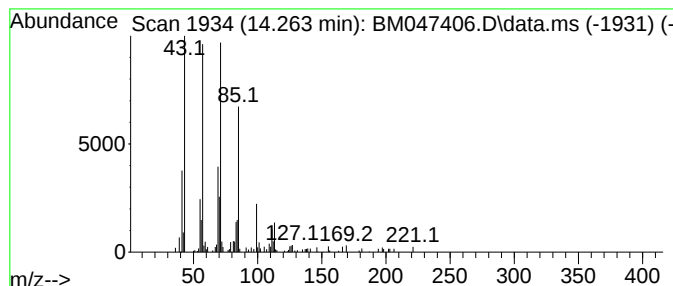
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Peak Number 2 Heptacosane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.263	2.02 ng	227257	Acenaphthene-d10	14.010

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Heptacosane	380	C27H56	000593-49-7	72
2		Disulfide, di-tert-dodecyl	402	C24H50S2	027458-90-8	64
3		Dodecane, 4,6-dimethyl-	198	C14H30	061141-72-8	64
4		Hexane, 2,4,4-trimethyl-	128	C9H20	016747-30-1	50
5		Succinic acid, 2-methylpent-3-yl...	286	C15H26O5	1010390-71-5	50



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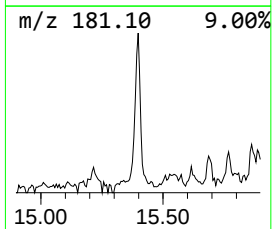
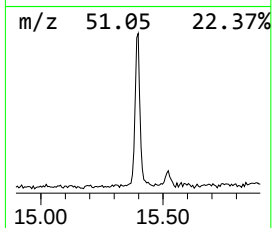
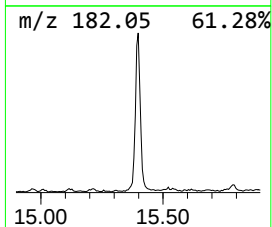
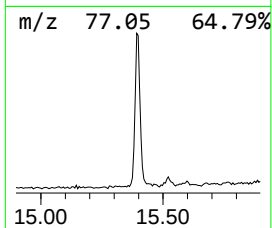
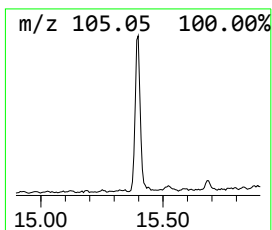
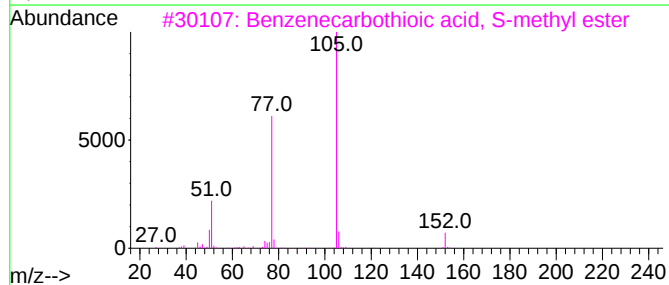
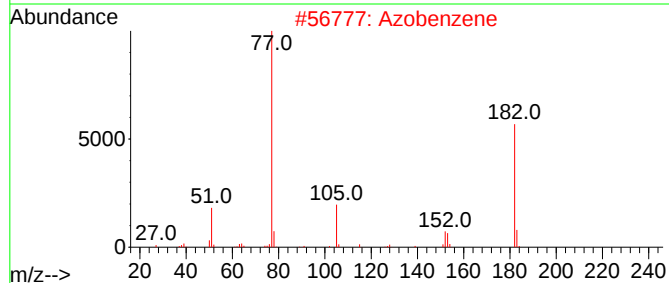
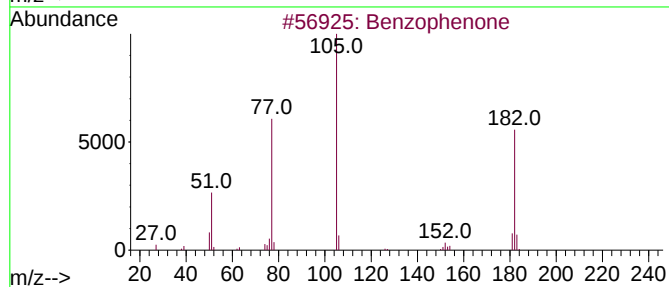
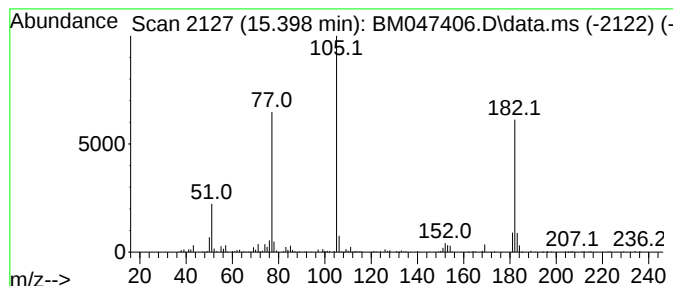
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Peak Number 3 Benzophenone Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.398	2.58 ng	312505	Phenanthrene-d10	16.774

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	97
2			Azobenzene	182	C12H10N2	000103-33-3	53
3			Benzenecarbothioic acid, S-methy...	152	C8H8OS	005925-68-8	49
4			1,2(4H)-Oxazine-3-ol, 5,6-dihydr...	219	C11H9N04	1000253-25-6	43
5			Phenylglyoxal	134	C8H6O2	001074-12-0	43



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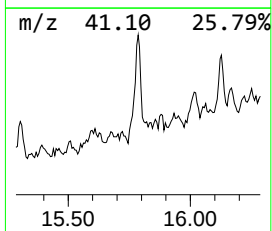
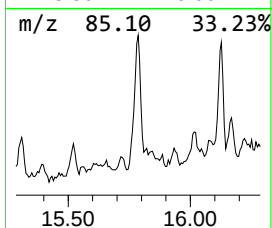
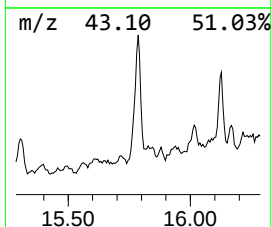
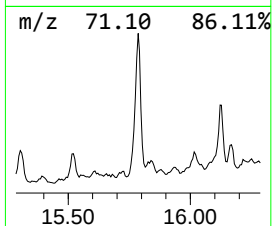
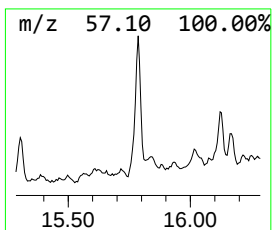
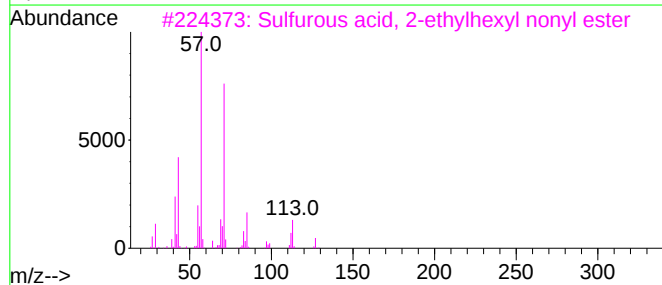
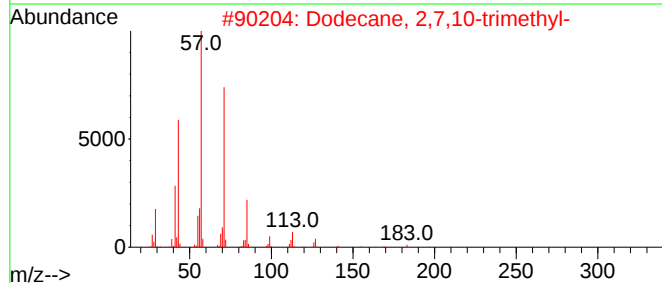
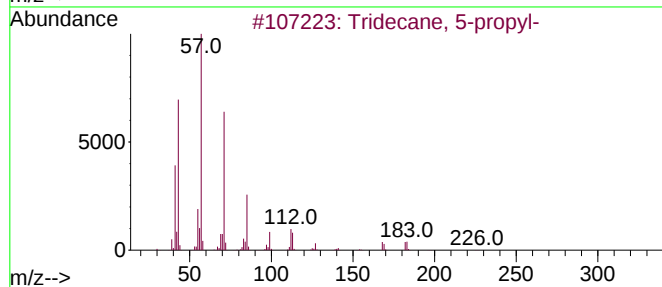
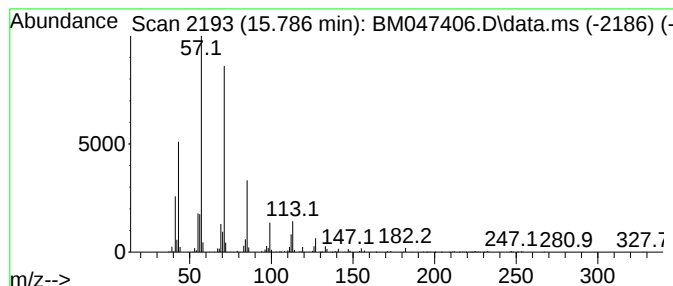
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Peak Number 4 Tridecane, 5-propyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.786	4.32 ng	524077	Phenanthrene-d10	16.774

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Tridecane, 5-propyl-	226	C16H34	055045-11-9	90
2		Dodecane, 2,7,10-trimethyl-	212	C15H32	074645-98-0	90
3		Sulfurous acid, 2-ethylhexyl non...	320	C17H36O3S	1010309-19-2	87
4		Sulfurous acid, decyl 2-ethylhex...	334	C18H38O3S	1000309-19-3	83
5		Tridecane, 3-ethyl-	212	C15H32	013286-73-2	83



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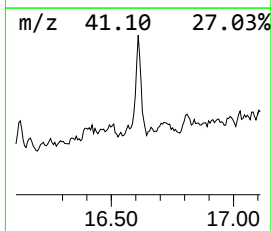
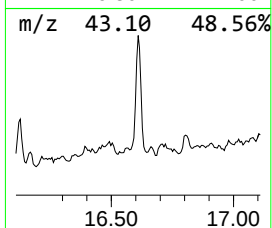
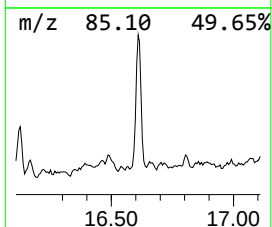
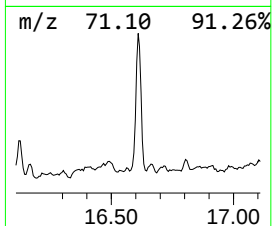
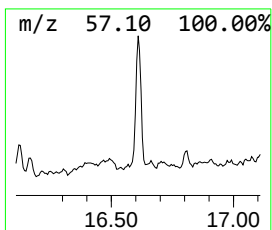
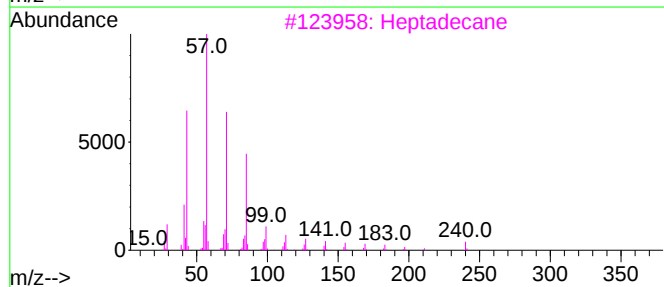
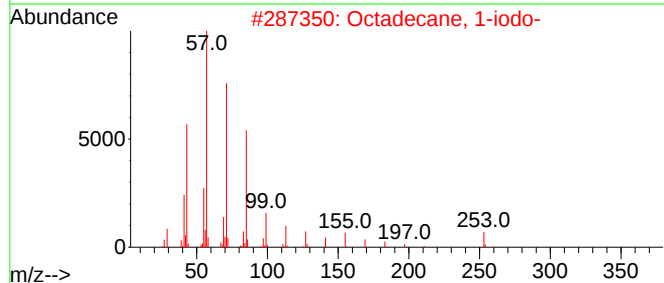
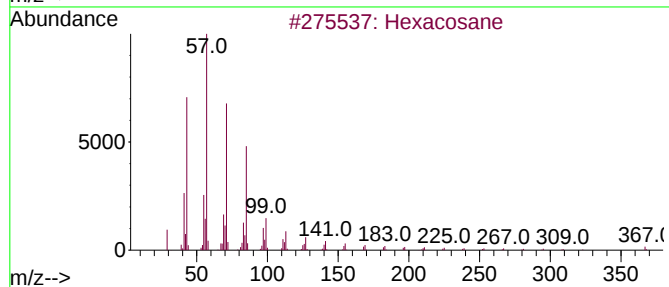
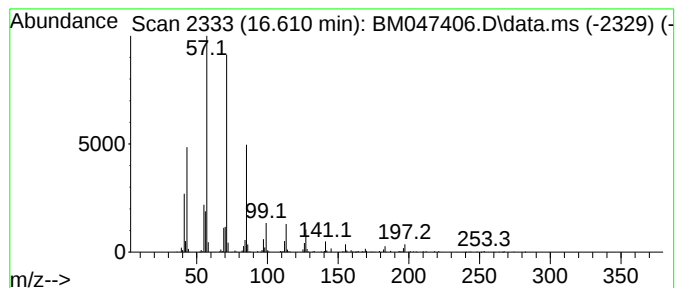
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Peak Number 5 Hexacosane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.610	7.07 ng	857965	Phenanthrene-d10	16.774

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexacosane	366	C26H54	000630-01-3	90
2			Octadecane, 1-iodo-	380	C18H37I	000629-93-6	90
3			Heptadecane	240	C17H36	000629-78-7	90
4			Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	86
5			3-Ethyl-2,6,10-trimethylundecane	226	C16H34	1000432-25-9	86



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CHRT-24376

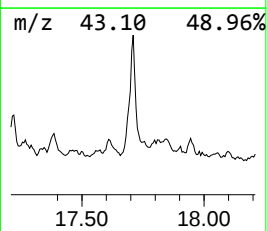
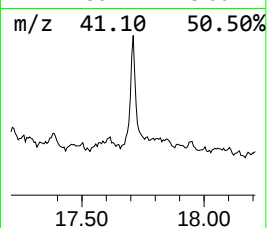
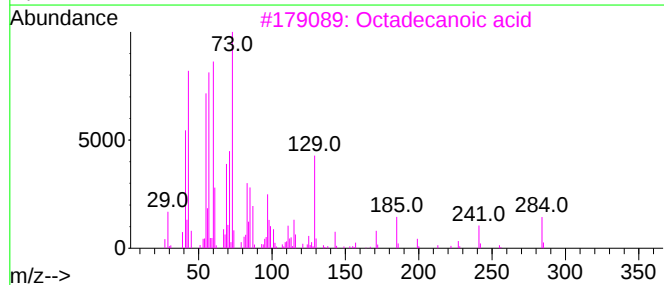
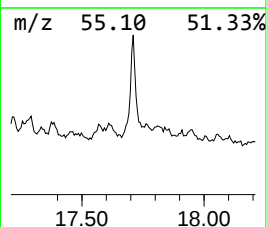
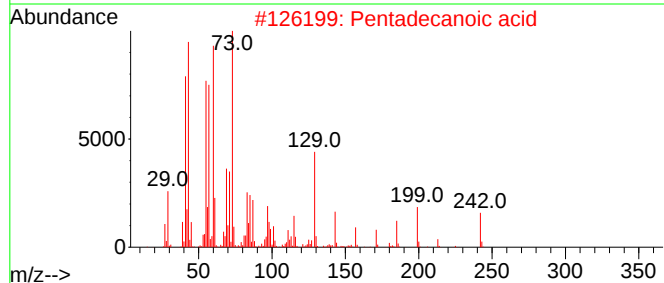
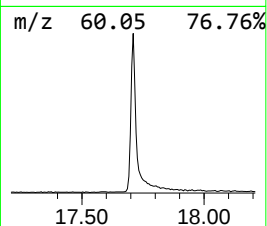
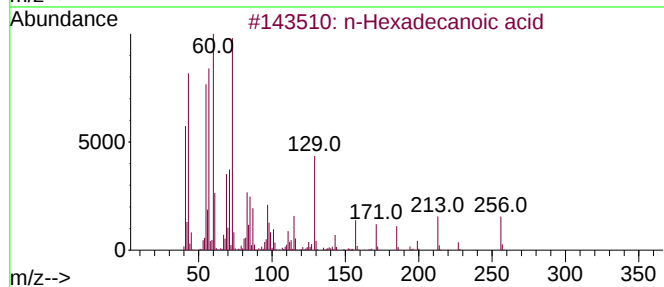
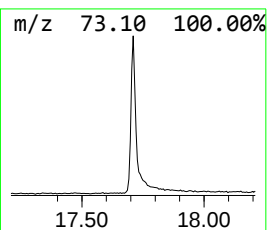
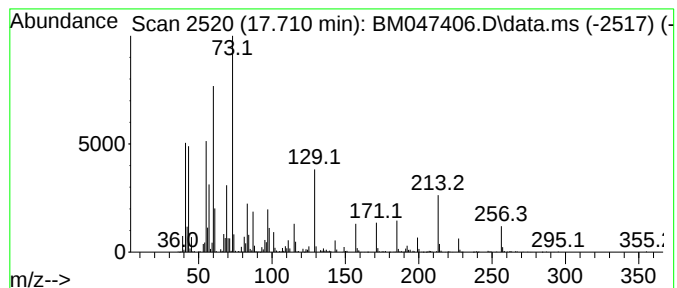
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.709	9.89 ng	1200170	Phenanthrene-d10	16.774

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	94
2		Pentadecanoic acid	242	C15H30O2	001002-84-2	72
3		Octadecanoic acid	284	C18H36O2	000057-11-4	59
4		n-Decanoic acid	172	C10H20O2	000334-48-5	58
5		Tridecanoic acid	214	C13H26O2	000638-53-9	53



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM083024\
Data File : BM047406.D
Acq On : 30 Aug 2024 15:00
Operator : RC/JU
Sample : P3794-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
CHRT-24376

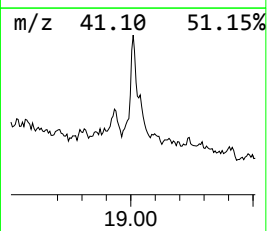
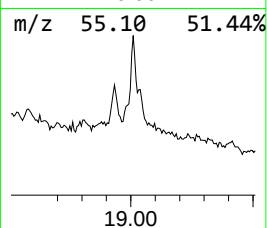
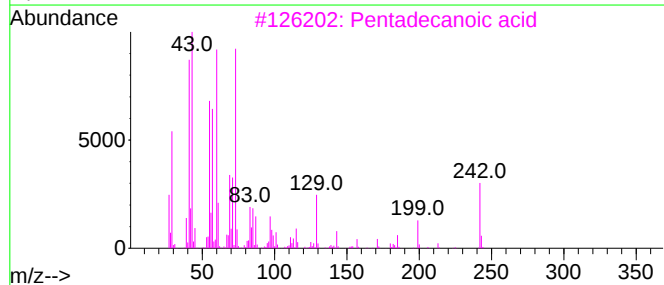
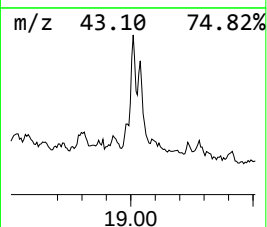
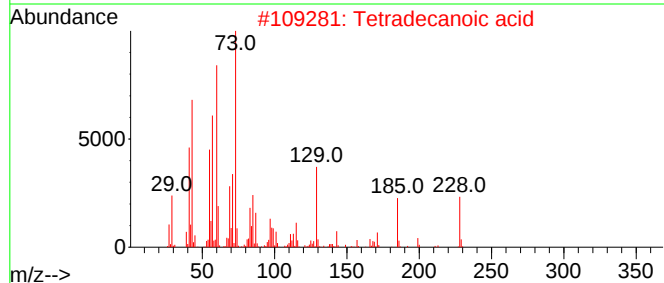
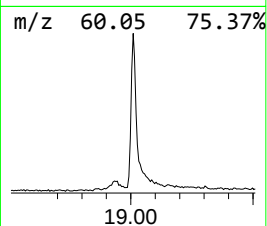
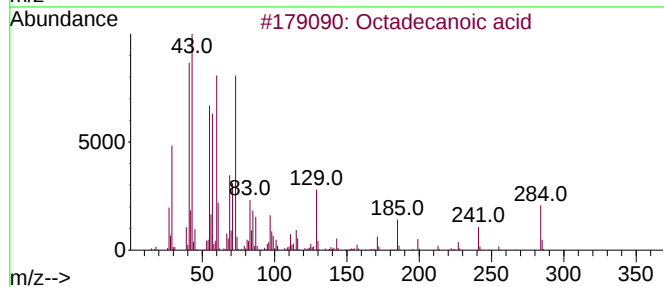
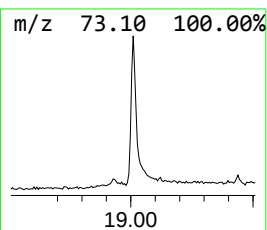
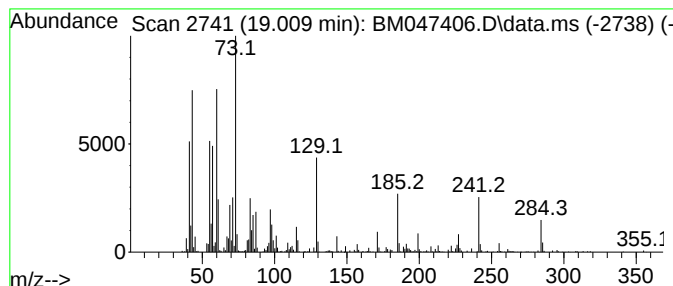
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Octadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.009	4.51 ng	492618	Chrysene-d12	21.021

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	97
2			Tetradecanoic acid	228	C14H28O2	000544-63-8	64
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	60
4			Dodecanoic acid	200	C12H24O2	000143-07-7	50
5			n-Decanoic acid	172	C10H20O2	000334-48-5	49



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM083024\
Data File : BM047406.D
Acq On : 30 Aug 2024 15:00
Operator : RC/JU
Sample : P3794-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
CHRT-24376

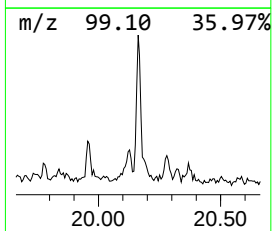
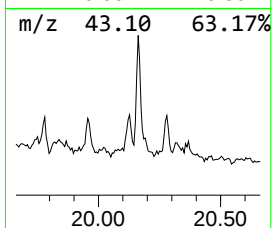
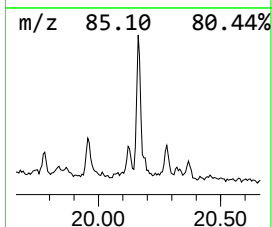
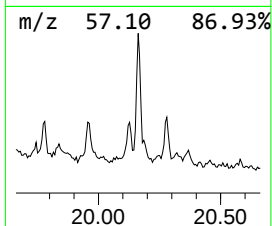
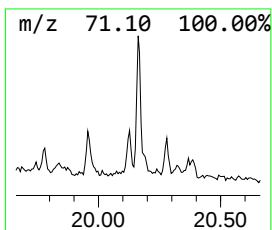
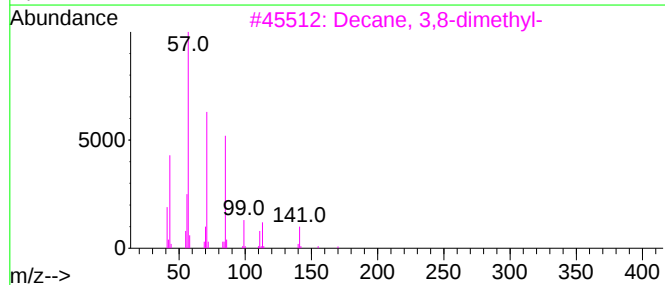
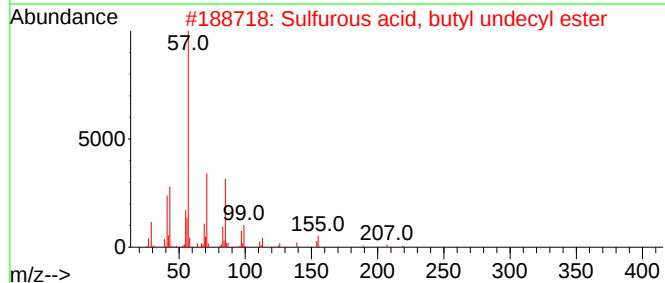
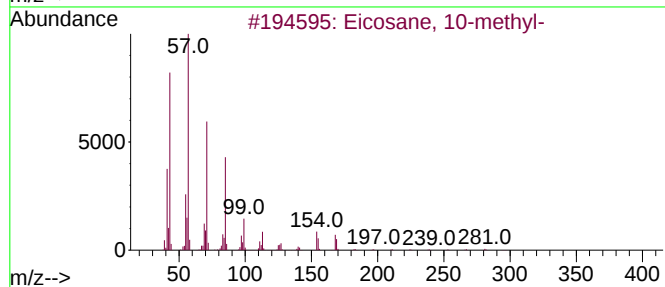
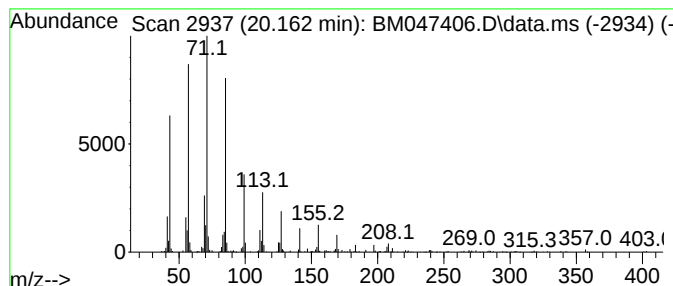
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Eicosane, 10-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.162	3.16 ng	345489	Chrysene-d12	21.021

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Eicosane, 10-methyl-	296	C21H44	054833-23-7	80
2			Sulfurous acid, butyl undecyl ester	292	C15H32O3S	1000309-17-8	72
3			Decane, 3,8-dimethyl-	170	C12H26	017312-55-9	72
4			Sulfurous acid, hexyl pentyl ester	236	C11H24O3S	1000309-14-1	50
5			Undecane, 4,8-dimethyl-	184	C13H28	017301-33-6	47



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM083024\
Data File : BM047406.D
Acq On : 30 Aug 2024 15:00
Operator : RC/JU
Sample : P3794-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
CHRT-24376

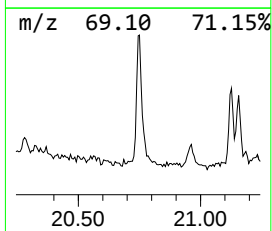
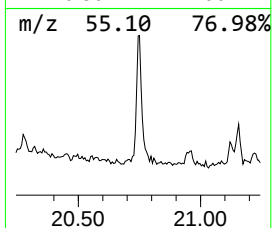
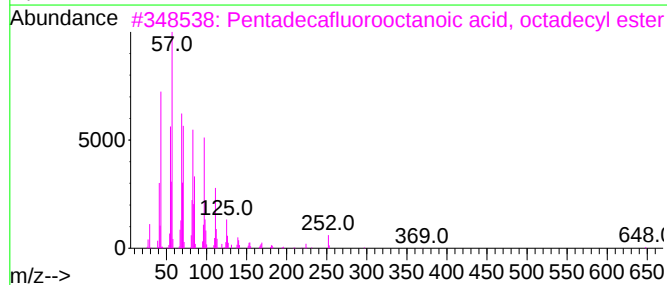
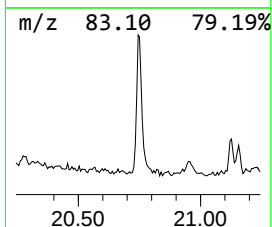
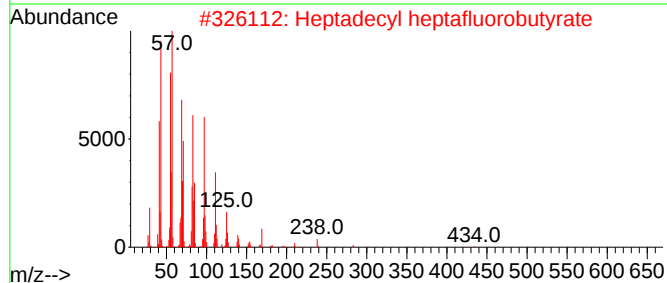
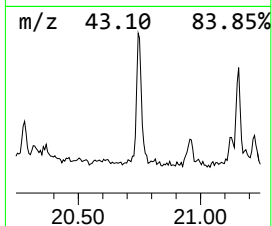
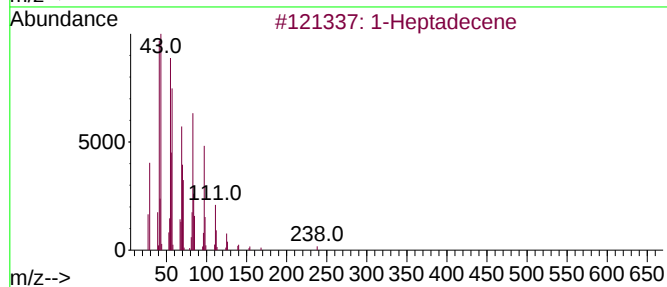
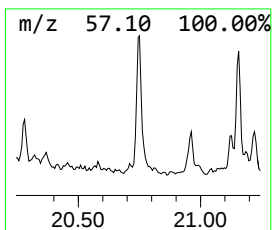
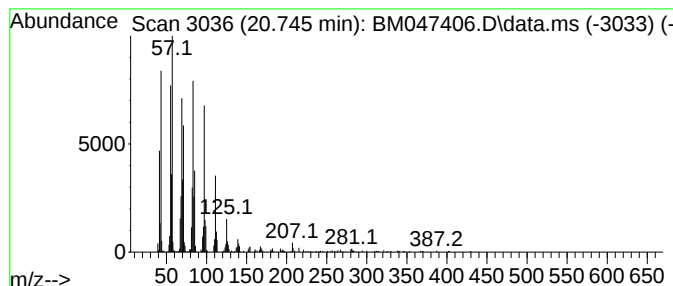
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 1-Heptadecene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.745	4.50 ng	491005	Chrysene-d12	21.021

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Heptadecene	238	C17H34	006765-39-5	95
2			Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94
3			Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	94
4			3-Eicosene, (E)-	280	C20H40	074685-33-9	92
5			Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM083024\
Data File : BM047406.D
Acq On : 30 Aug 2024 15:00
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Sample : P3794-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
CHRT-24376

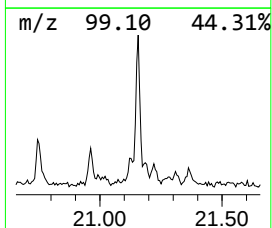
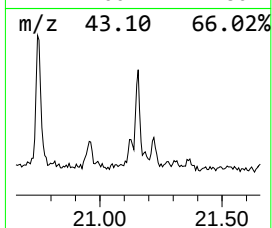
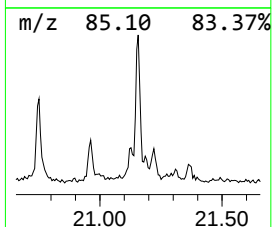
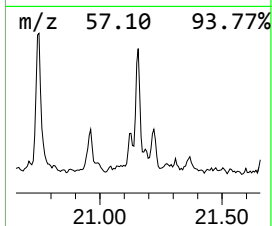
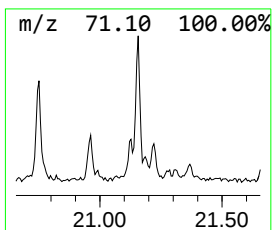
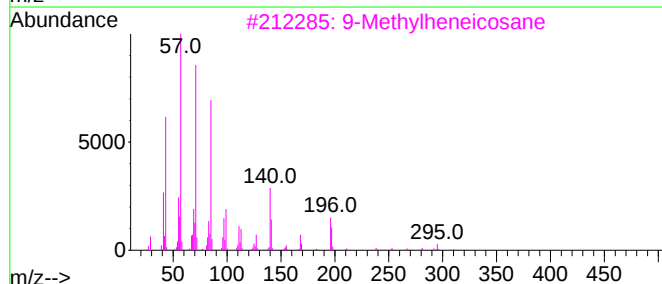
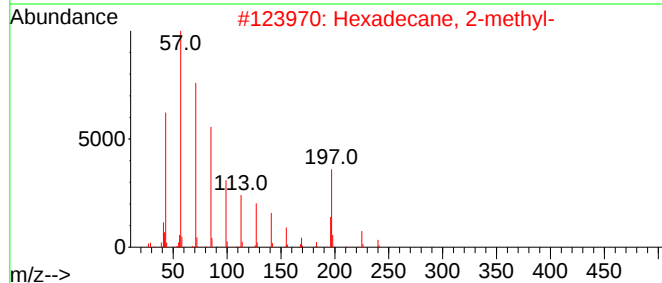
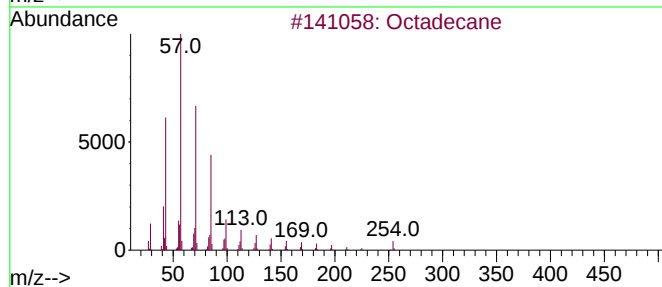
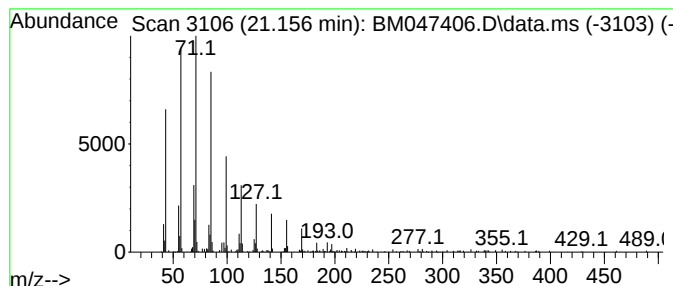
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Octadecane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.156	2.30 ng	250639	Chrysene-d12	21.021

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Octadecane	254	C18H38	000593-45-3	90
2		Hexadecane, 2-methyl-	240	C17H36	001560-92-5	78
3		9-Methylheneicosane	310	C22H46	070475-51-3	58
4		Tridecane, 1-iodo-	310	C13H27I	035599-77-0	52
5		Sulfurous acid, hexyl pentyl ester	236	C11H24O3S	1000309-14-1	46



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM083024\
Data File : BM047406.D
Acq On : 30 Aug 2024 15:00
Operator : RC/JU
Sample : P3794-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
CHRT-24376

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM082624.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
2-Pentanone, 4-...	4.557	3.7	ng	234742	1	7.345	1259770	20.0
Heptacosane	14.263	2.0	ng	227257	3	14.010	2245760	20.0
Benzophenone	15.398	2.6	ng	312505	4	16.774	2426370	20.0
Tridecane, 5-pr...	15.786	4.3	ng	524077	4	16.774	2426370	20.0
Hexacosane	16.610	7.1	ng	857965	4	16.774	2426370	20.0
n-Hexadecanoic ...	17.709	9.9	ng	1200170	4	16.774	2426370	20.0
Octadecanoic acid	19.009	4.5	ng	492618	5	21.021	2183450	20.0
Eicosane, 10-me...	20.162	3.2	ng	345489	5	21.021	2183450	20.0
1-Heptadecene	20.745	4.5	ng	491005	5	21.021	2183450	20.0
Octadecane	21.156	2.3	ng	250639	5	21.021	2183450	20.0