

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF022525\
 Data File : BF141761.D
 Acq On : 25 Feb 2025 13:37
 Operator : RC/JU
 Sample : Q1421-01
 Misc :
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 P001-CLAY-CF01-01

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_F\Methods\8270-BF020625.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF141761.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.987	488	492	510	rVB	38197	66431	3.15%	0.407%
2	5.404	558	563	588	rBV	1176006	1716581	81.35%	10.524%
3	6.422	731	736	765	rBV	1204425	1783529	84.52%	10.934%
4	6.781	792	797	805	rBV	339285	424257	20.10%	2.601%
5	7.345	887	893	904	rBV	819392	1114602	52.82%	6.833%
6	7.604	933	937	951	rBV	21244	46123	2.19%	0.283%
7	8.063	1009	1015	1034	rBV	407651	565496	26.80%	3.467%
8	9.133	1192	1197	1209	rBV	1623877	2110220	100.00%	12.937%
9	9.816	1307	1313	1326	rBV	463314	627750	29.75%	3.848%
10	10.527	1429	1434	1442	rVB	217247	279253	13.23%	1.712%
11	10.604	1442	1447	1461	rBV	792838	1074751	50.93%	6.589%
12	11.298	1560	1565	1580	rBV	430185	596483	28.27%	3.657%
13	11.833	1648	1656	1680	rBV	650947	1253018	59.38%	7.682%
14	12.074	1694	1697	1704	rVB4	16003	21888	1.04%	0.134%
15	12.345	1733	1743	1756	rVB3	34516	129227	6.12%	0.792%
16	12.539	1769	1776	1782	rBV5	28081	71466	3.39%	0.438%
17	12.615	1783	1789	1801	rVV	228286	457712	21.69%	2.806%
18	12.810	1813	1822	1829	rBV	120576	313863	14.87%	1.924%
19	12.880	1829	1834	1840	rVB	1342775	1747980	82.83%	10.716%
20	13.239	1887	1895	1903	rBV	55282	119248	5.65%	0.731%
21	13.798	1983	1990	1998	rBV4	32235	109912	5.21%	0.674%
22	13.880	1998	2004	2009	rVV	77211	154879	7.34%	0.950%
23	13.939	2009	2014	2028	rVB	319717	464226	22.00%	2.846%
24	14.092	2036	2040	2046	rBV	24779	38059	1.80%	0.233%
25	14.404	2087	2093	2106	rBV	97028	194181	9.20%	1.190%
26	14.692	2137	2142	2149	rBV3	58107	110028	5.21%	0.675%
27	14.892	2171	2176	2182	rBV	50321	101942	4.83%	0.625%
28	15.027	2194	2199	2208	rVB	39880	64722	3.07%	0.397%
29	15.386	2254	2260	2266	rBV	294021	507231	24.04%	3.110%
30	15.815	2329	2333	2341	rVB	25614	46575	2.21%	0.286%

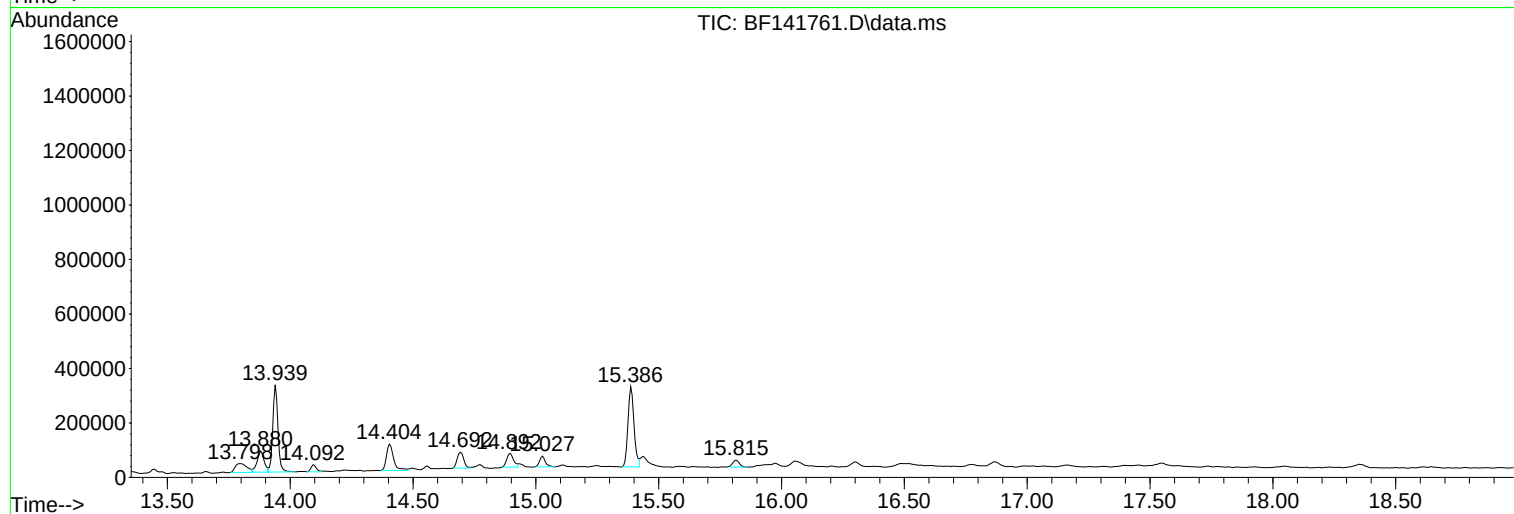
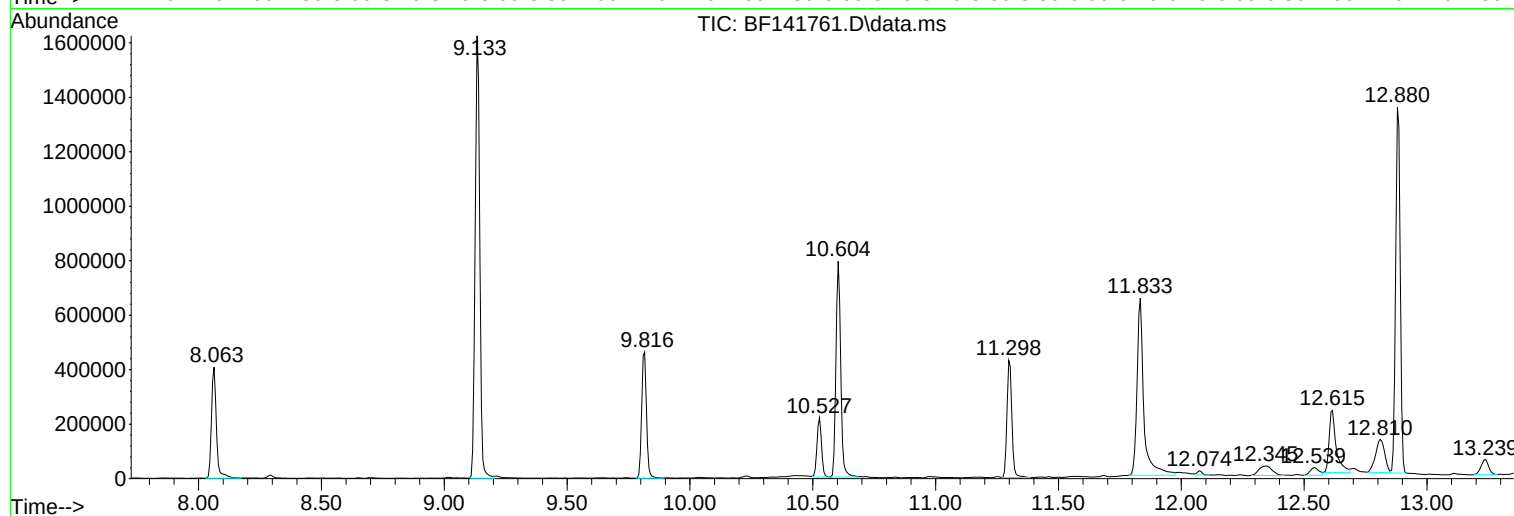
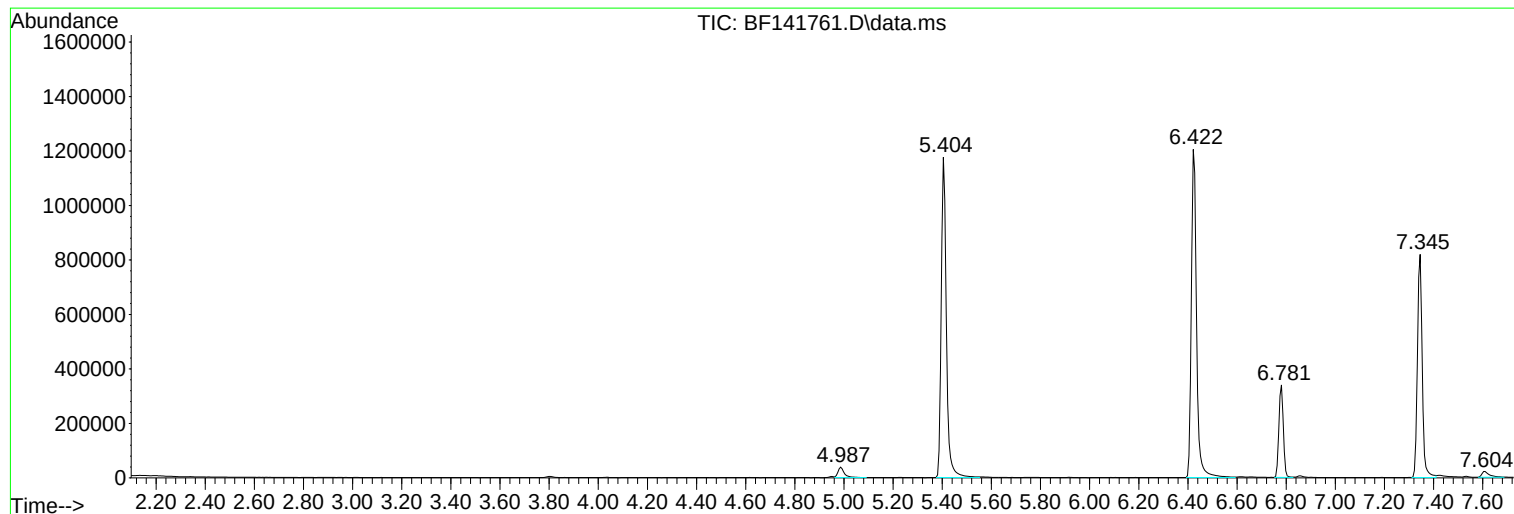
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF020625.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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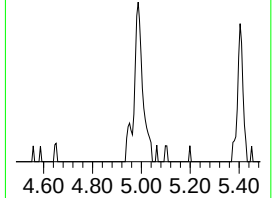
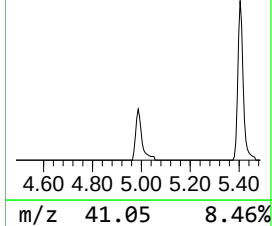
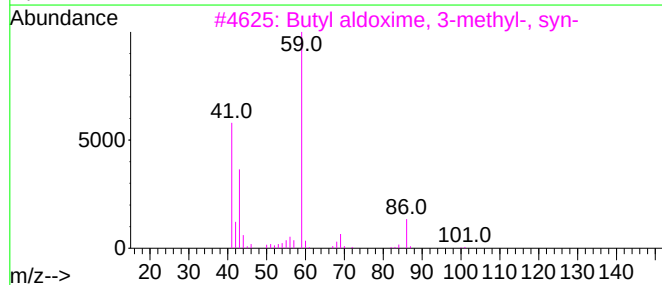
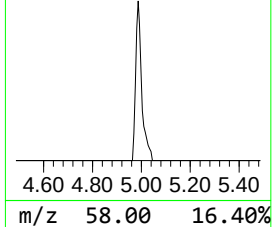
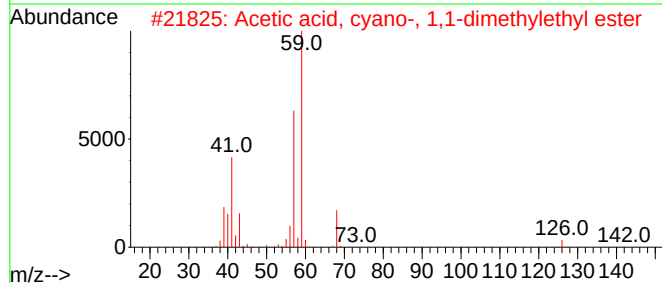
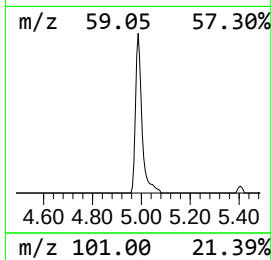
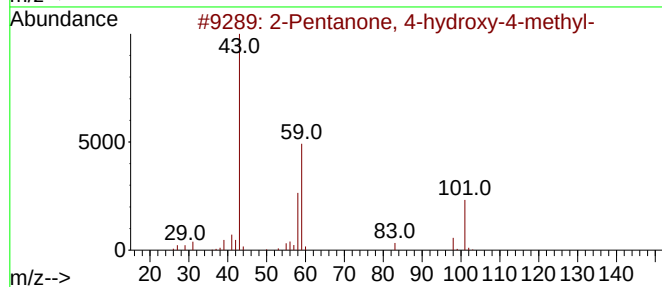
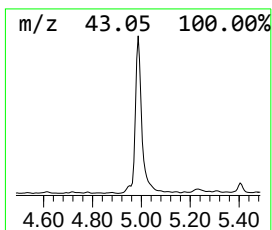
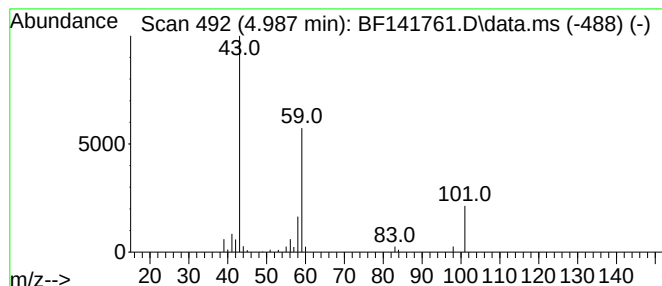
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.987	3.13 ng	66431	1,4-Dichlorobenzene-d4	6.781

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, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23		
3	Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	17		
4	Acetone	58	C3H6O	000067-64-1	10		
5	Silane, trimethyl-	74	C3H10Si	000993-07-7	9		



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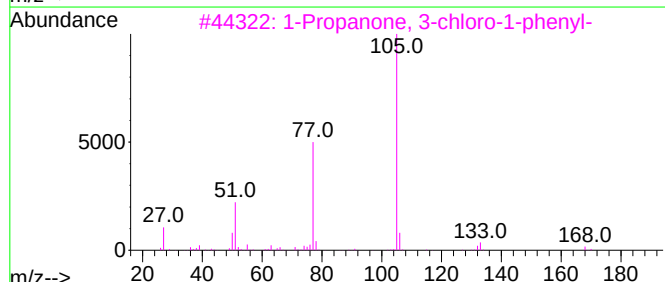
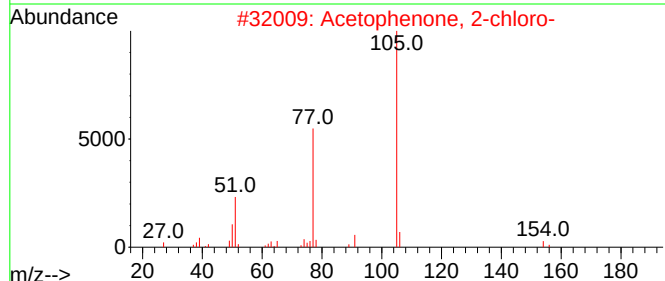
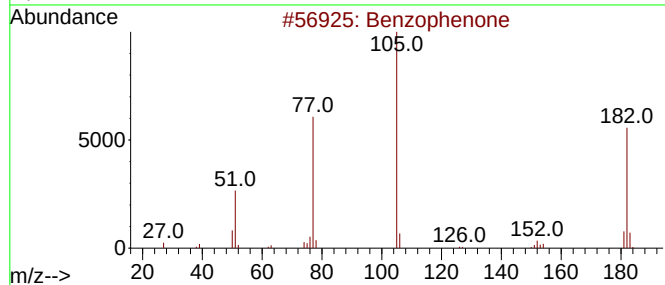
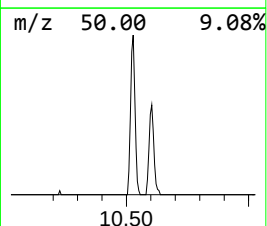
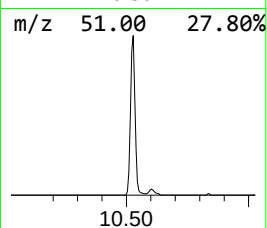
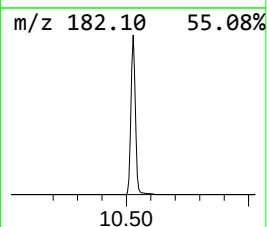
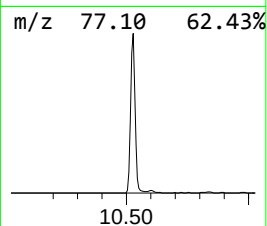
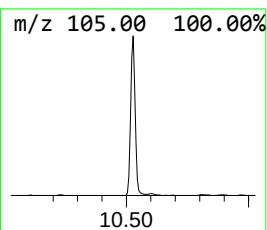
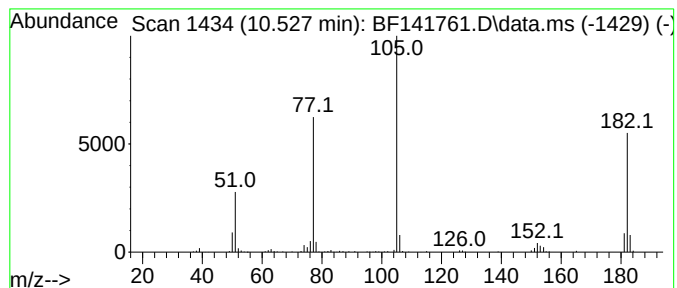
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TIC Library : C:\Database\NIST20.L
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Peak Number 2 Benzophenone Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.527	8.90 ng	279253	Acenaphthene-d10	9.816

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	96
2			Acetophenone, 2-chloro-	154	C8H7ClO	000532-27-4	52
3			1-Propanone, 3-chloro-1-phenyl-	168	C9H9ClO	000936-59-4	50
4			1-Propanone, 2-bromo-1-phenyl-	212	C9H9BrO	002114-00-3	50
5			Pentafluoroethyl phenyl ketone	224	C9H5F5O	000394-52-5	50



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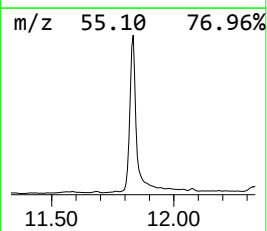
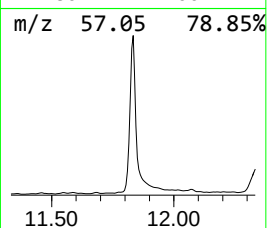
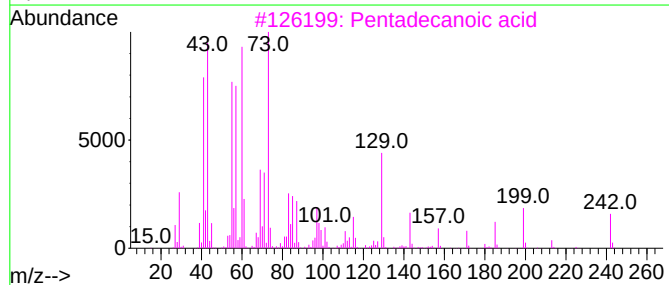
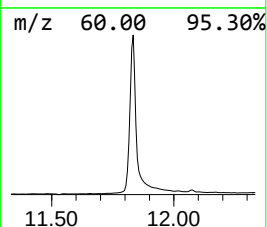
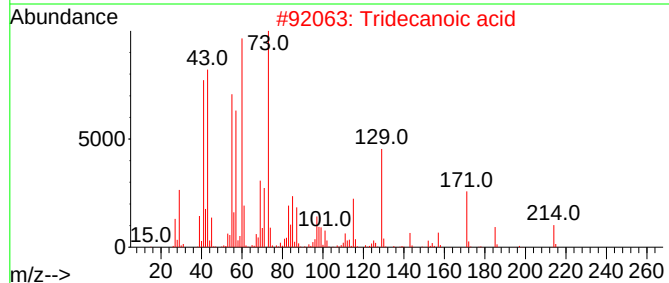
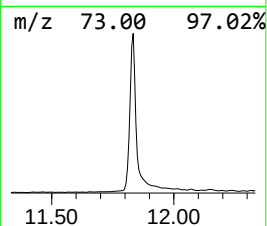
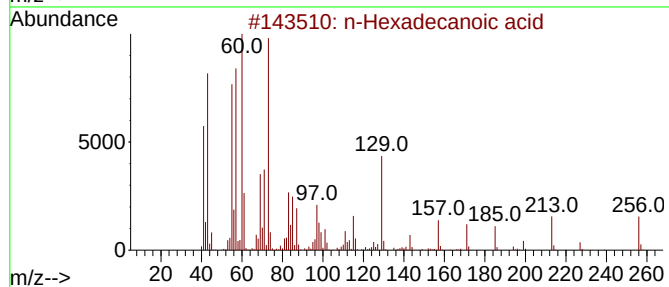
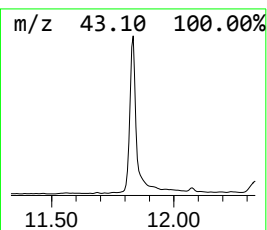
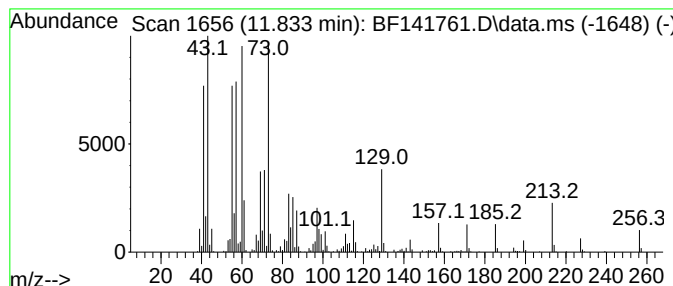
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.833	42.01 ng	1253020	Phenanthrene-d10	11.298

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Tridecanoic acid	214	C13H26O2	000638-53-9	94
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	91
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	83
5			n-Decanoic acid	172	C10H20O2	000334-48-5	64



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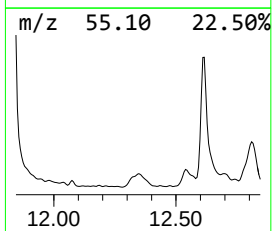
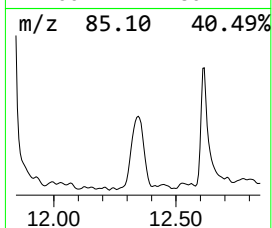
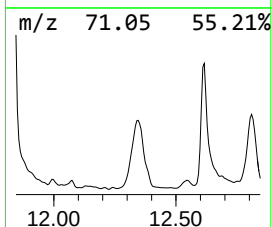
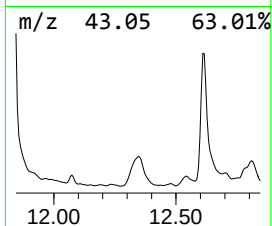
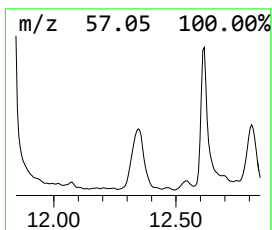
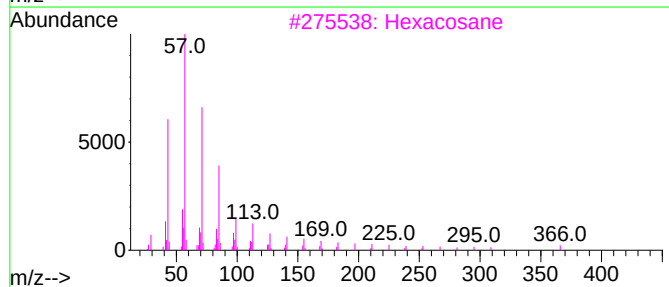
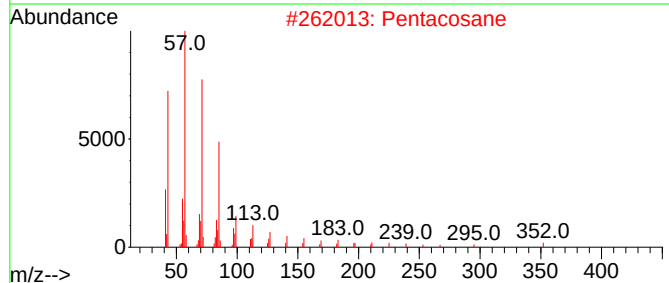
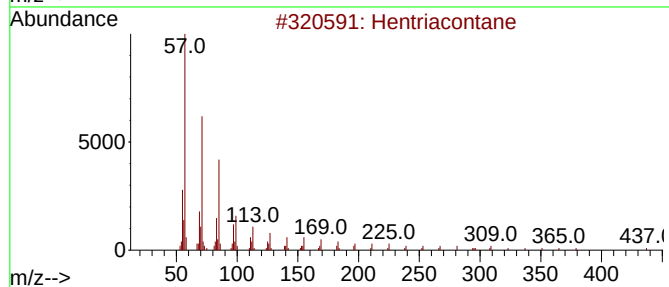
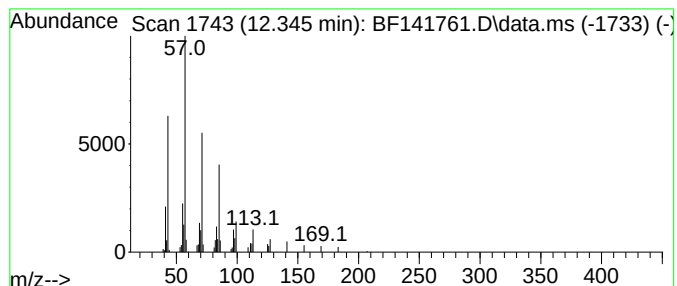
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 Hentriacontane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.345	4.33 ng	129227	Phenanthrene-d10	11.298

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hentriacontane	437	C31H64	000630-04-6	91
2			Pentacosane	352	C25H52	000629-99-2	91
3			Hexacosane	366	C26H54	000630-01-3	91
4			Heneicosane	296	C21H44	000629-94-7	91
5			Heptadecane	240	C17H36	000629-78-7	91



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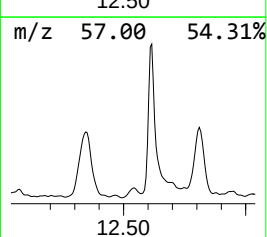
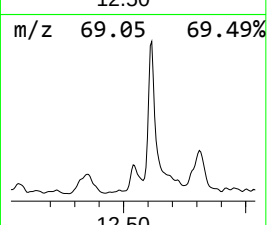
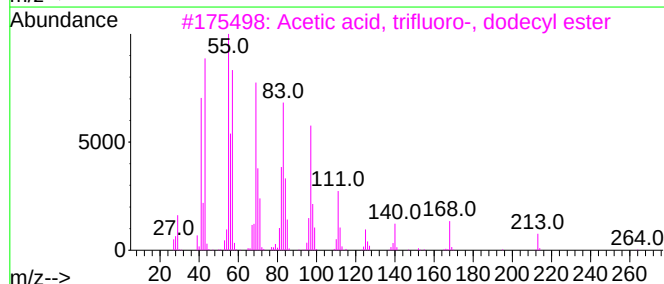
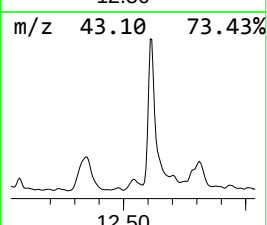
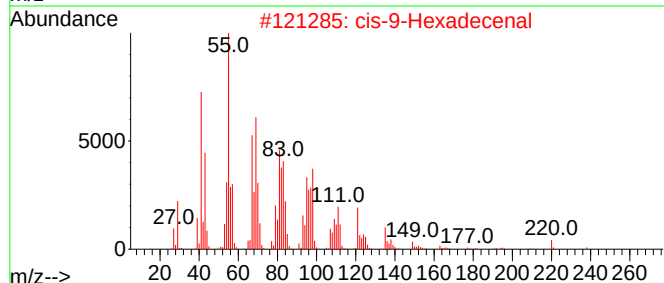
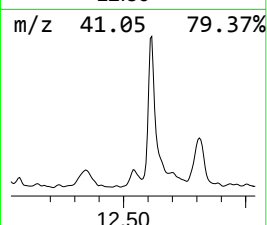
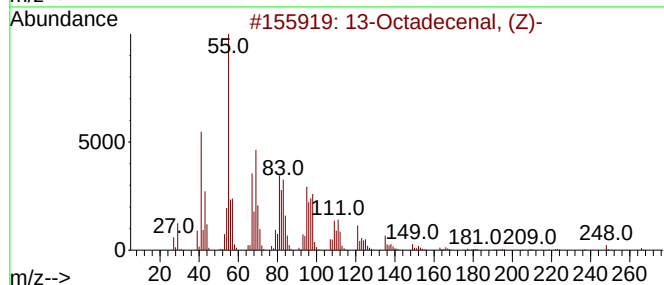
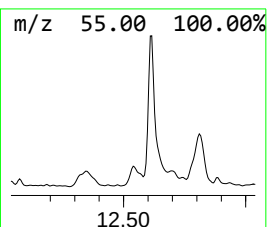
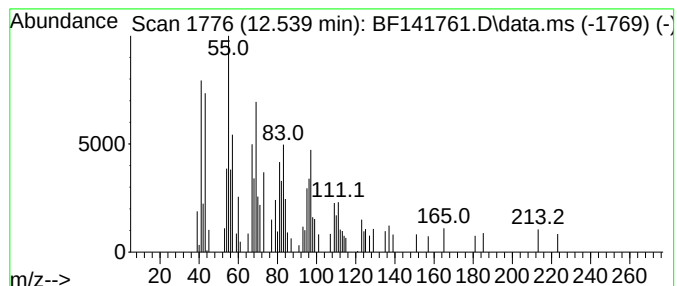
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 13-Octadecenal, (Z)- Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.539	2.40 ng	71466	Phenanthrene-d10	11.298

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			13-Octadecenal, (Z)-	266	C18H34O	058594-45-9	64
2			cis-9-Hexadecenal	238	C16H30O	056219-04-6	62
3			Acetic acid, trifluoro-, dodecyl...	282	C14H25F3O2	006222-00-0	50
4			8-Oxabicyclo[5.1.0]octane	112	C7H12O	000286-45-3	50
5			13-Tetradecenal	210	C14H26O	085896-31-7	49



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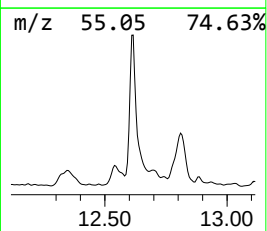
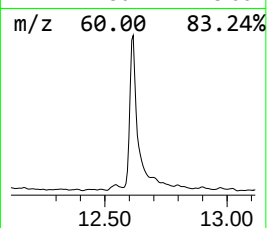
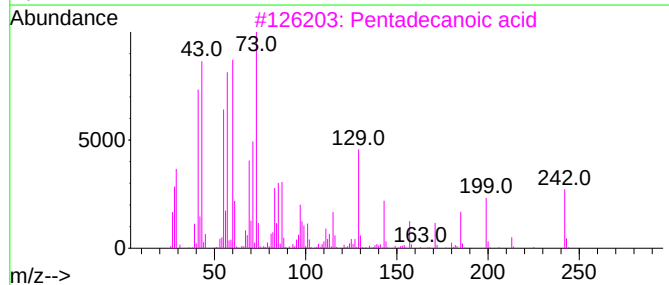
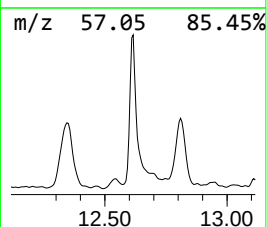
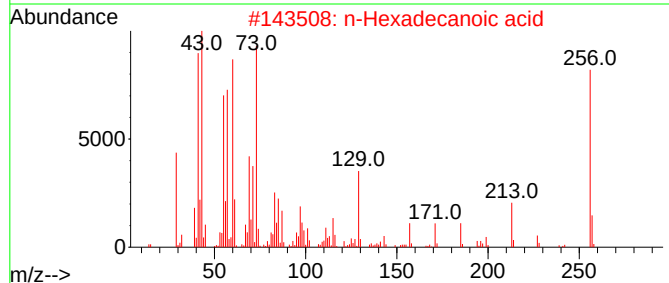
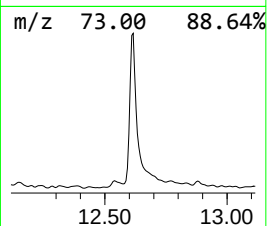
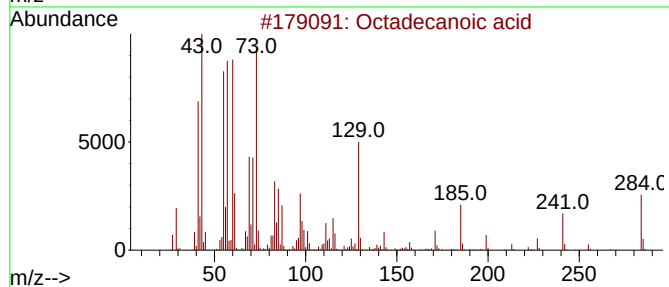
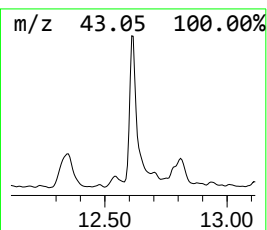
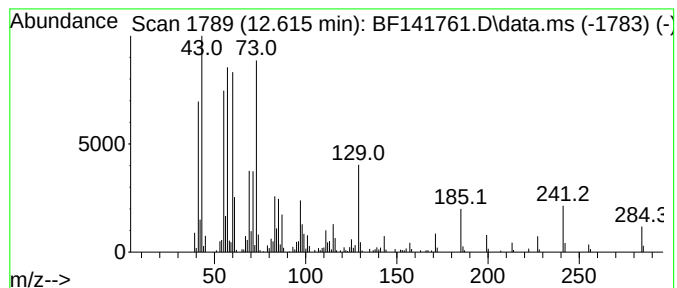
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Octadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.616	15.35 ng	457712	Phenanthrene-d10	11.298

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	99
2			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	89
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	89
4			n-Decanoic acid	172	C10H20O2	000334-48-5	78
5			Tridecanoic acid	214	C13H26O2	000638-53-9	70



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF022525\
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Acq On : 25 Feb 2025 13:37
Operator : RC/JU
Sample : Q1421-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

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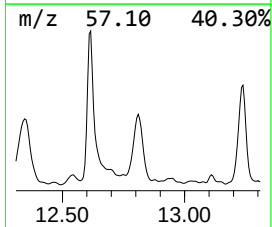
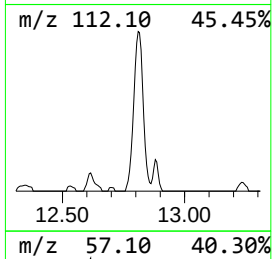
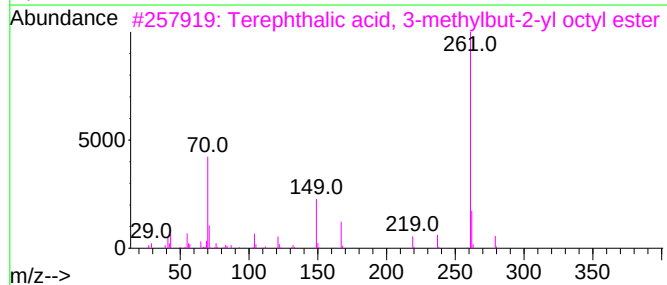
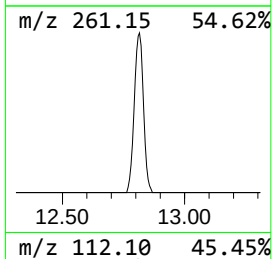
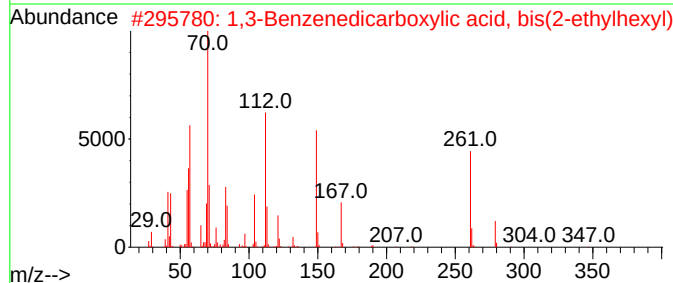
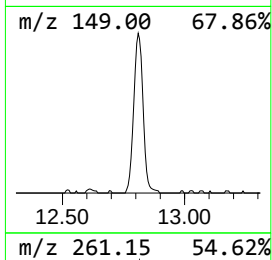
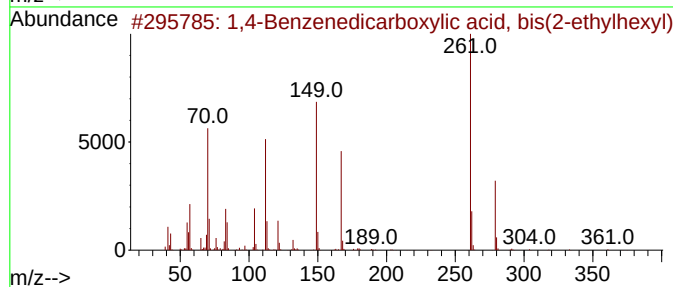
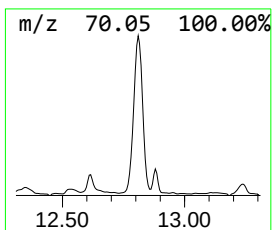
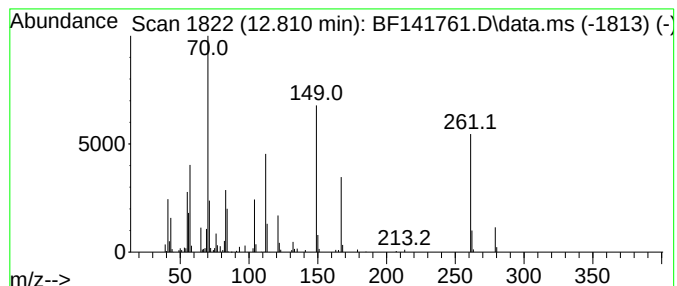
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 1,4-Benzenedicarboxylic aci... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.810	13.52 ng	313863	Chrysene-d12	13.939

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,4-Benzenedicarboxylic acid, bi...	390	C24H38O4	006422-86-2	74
2			1,3-Benzenedicarboxylic acid, bi...	390	C24H38O4	000137-89-3	64
3			Terephthalic acid, 3-methylbut-2...	348	C21H32O4	1000356-27-6	53
4			Terephthalic acid, monochloride,...	296	C16H21ClO3	1000324-22-9	43
5			Bromoacetic acid, 2-ethylhexyl e...	250	C10H19BrO2	068144-73-0	35



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF022525\
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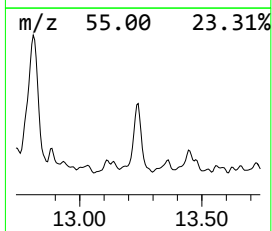
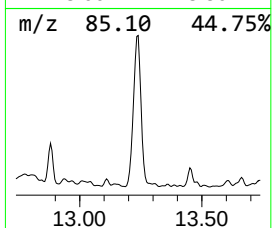
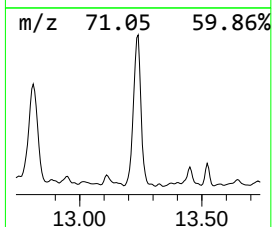
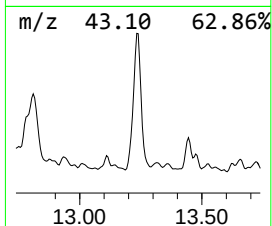
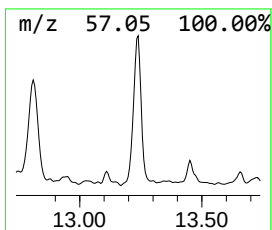
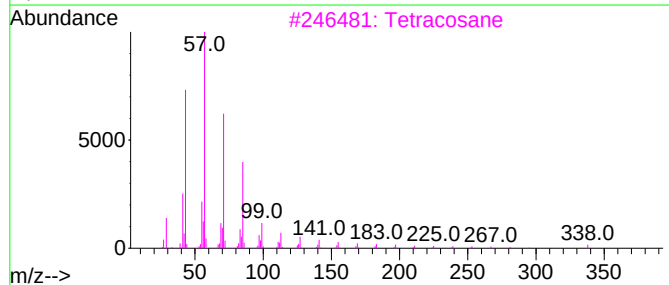
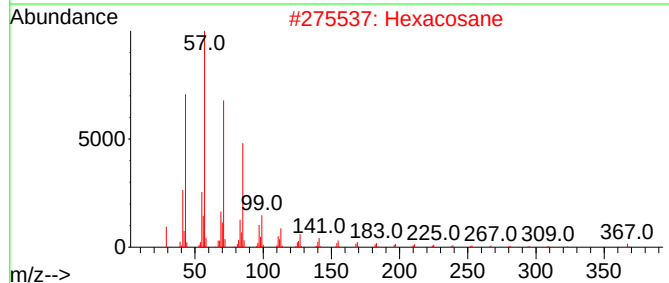
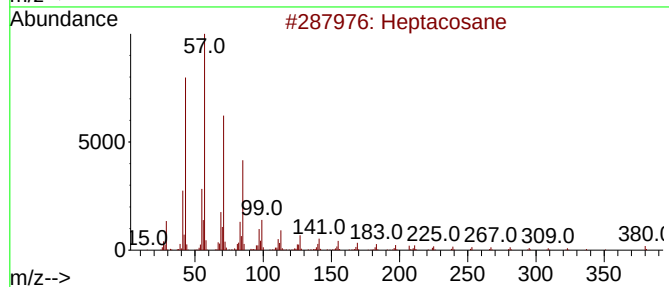
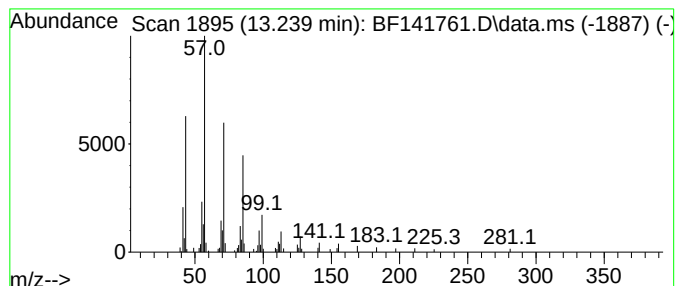
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Heptacosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.239	5.14 ng	119248	Chrysene-d12	13.939

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Heptacosane	380	C27H56	000593-49-7	91
2		Hexacosane	366	C26H54	000630-01-3	91
3		Tetracosane	338	C24H50	000646-31-1	91
4		Octacosane	394	C28H58	000630-02-4	91
5		Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF022525\
Data File : BF141761.D
Acq On : 25 Feb 2025 13:37
Operator : RC/JU
Sample : Q1421-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

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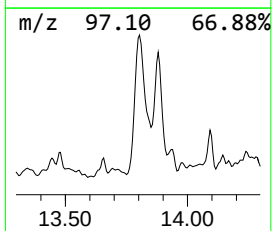
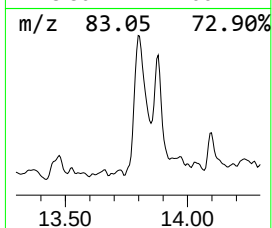
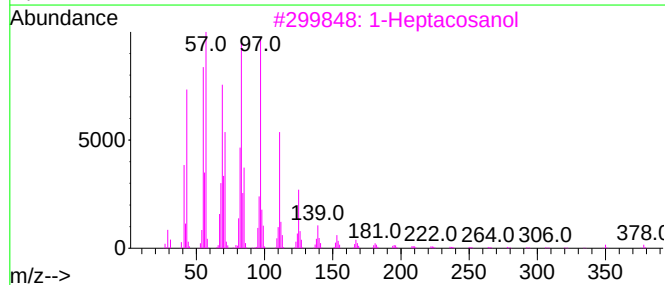
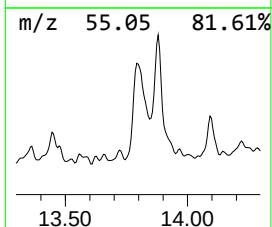
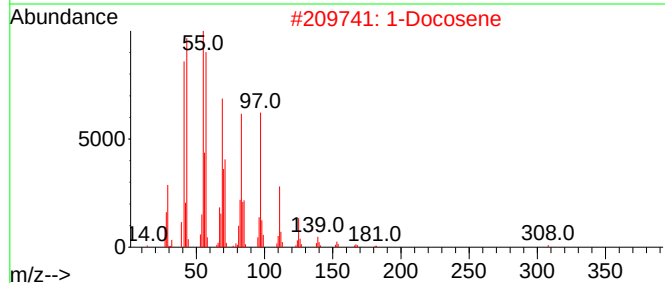
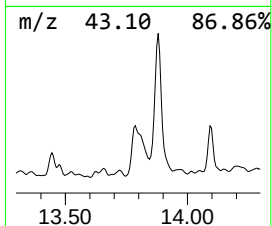
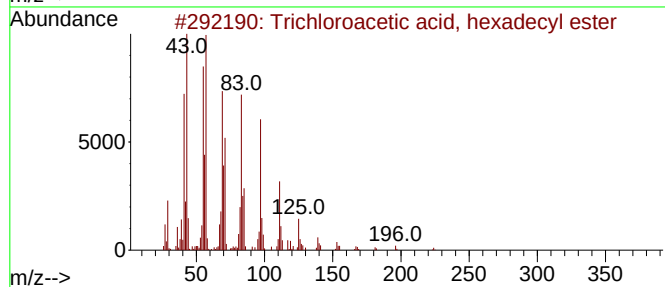
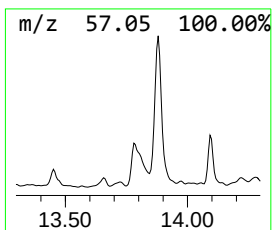
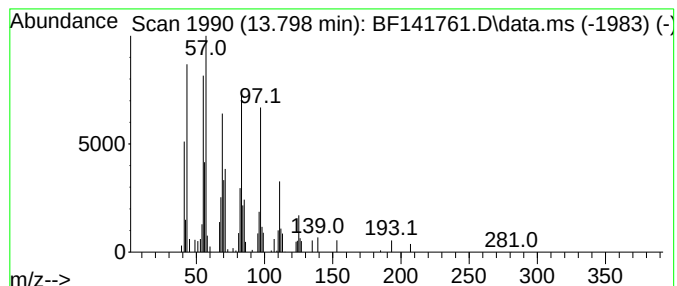
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Trichloroacetic acid, hexad... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.798	4.74 ng	109912	Chrysene-d12	13.939

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	94
2			1-Docosene	308	C22H44	001599-67-3	94
3			1-Heptacosanol	396	C27H56O	002004-39-9	93
4			n-Tetracosanol-1	354	C24H50O	000506-51-4	93
5			1-Hexacosene	364	C26H52	018835-33-1	93



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF022525\
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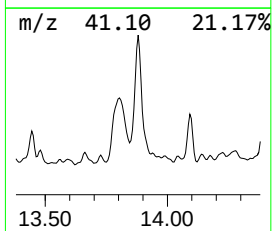
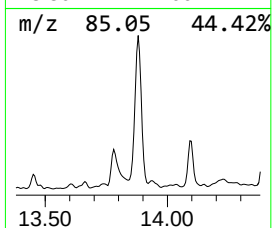
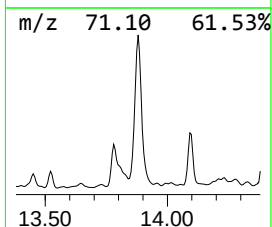
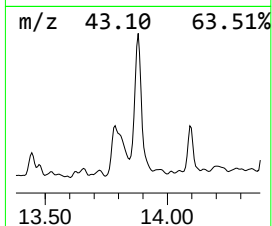
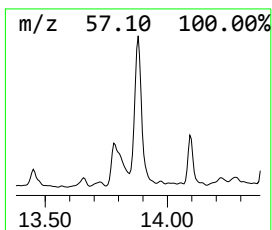
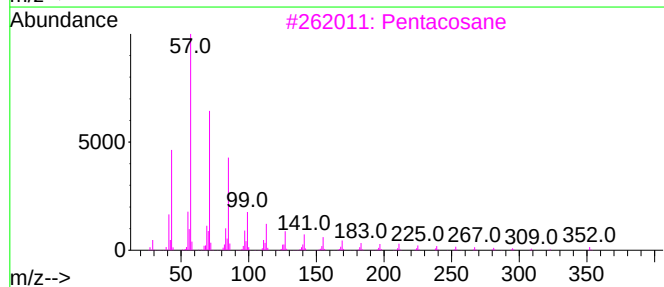
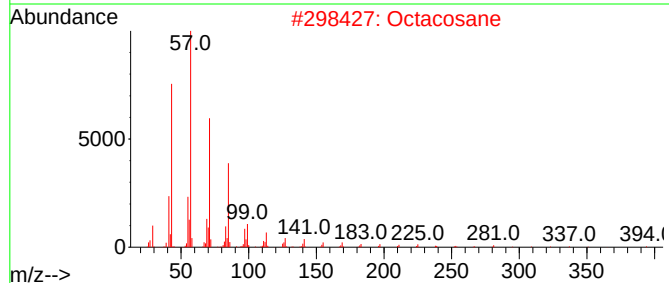
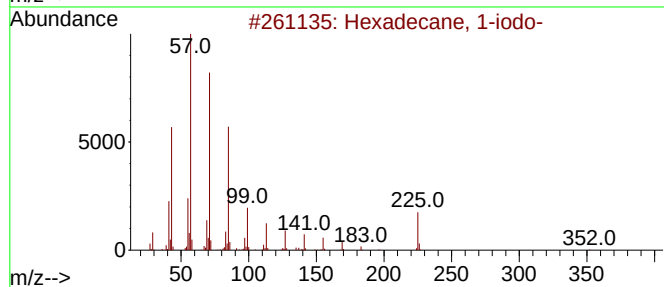
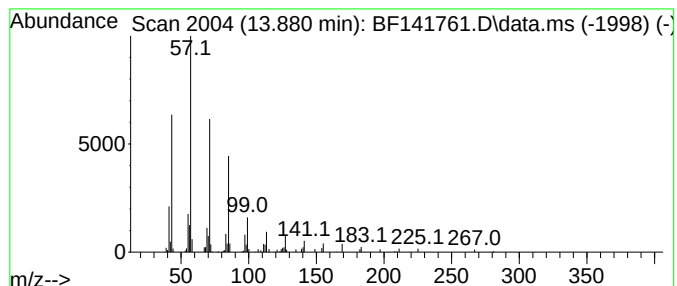
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Hexadecane, 1-iodo- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.880	6.67 ng	154879	Chrysene-d12	13.939

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Hexadecane, 1-iodo-	352	C16H33I	000544-77-4	91
2		Octacosane	394	C28H58	000630-02-4	91
3		Pentacosane	352	C25H52	000629-99-2	91
4		Octadecane	254	C18H38	000593-45-3	90
5		Docosane	310	C22H46	000629-97-0	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF022525\
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Operator : RC/JU
Sample : Q1421-01
Misc :
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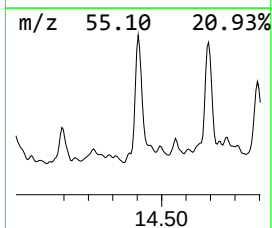
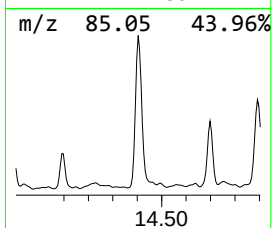
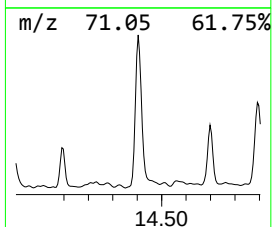
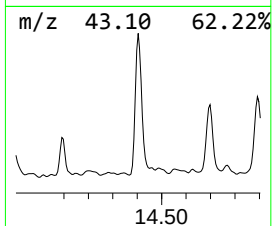
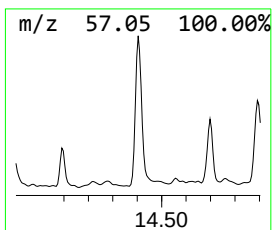
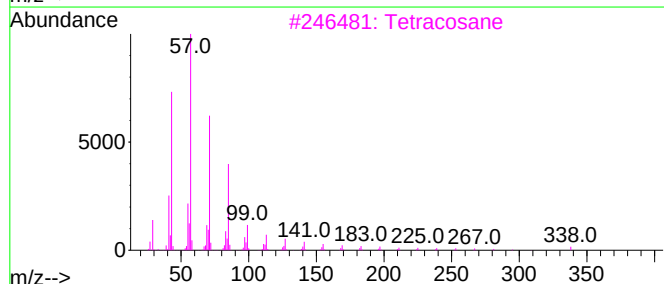
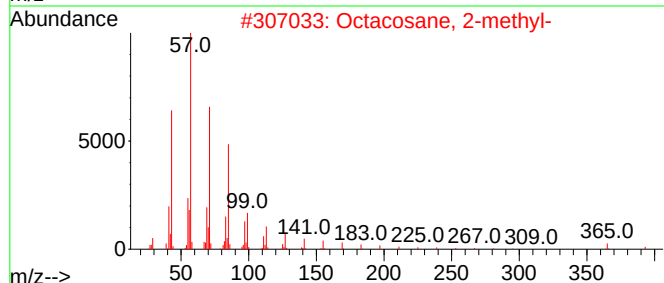
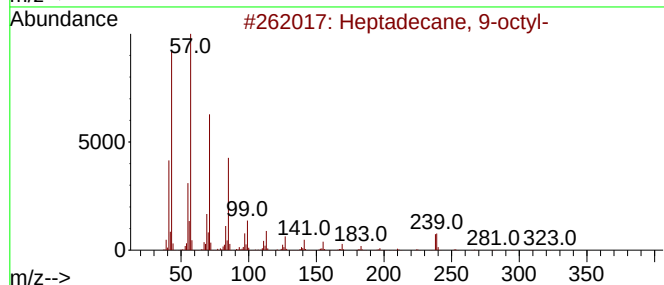
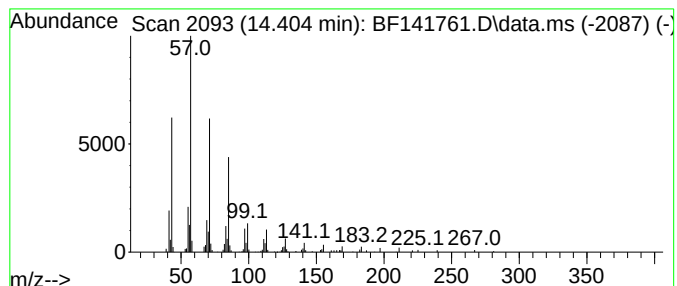
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Heptadecane, 9-octyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.404	8.37 ng	194181	Chrysene-d12	13.939	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
2	Octacosane, 2-methyl-	408	C29H60	001560-98-1	91
3	Tetracosane	338	C24H50	000646-31-1	91
4	Heptacosane	380	C27H56	000593-49-7	91
5	Heneicosane	296	C21H44	000629-94-7	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF022525\
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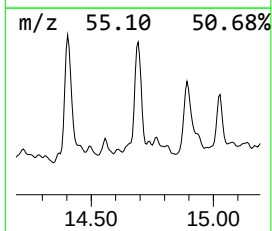
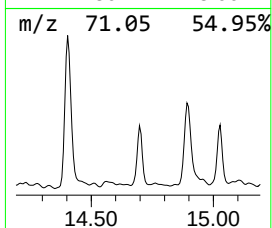
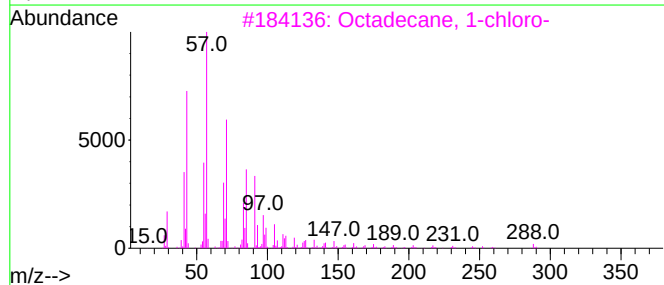
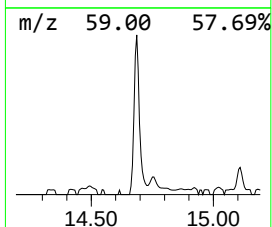
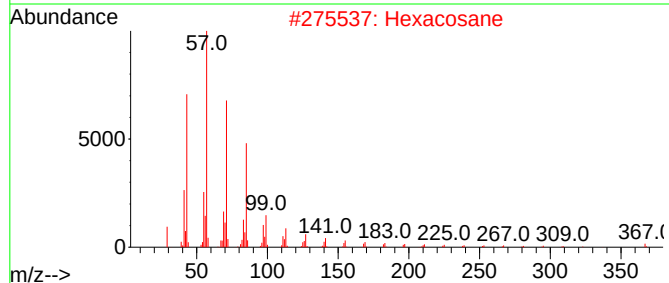
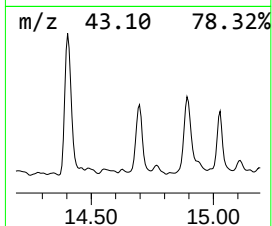
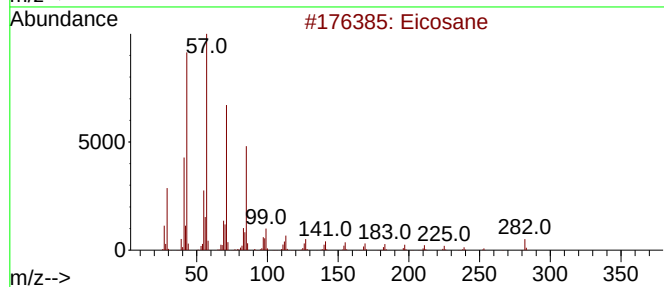
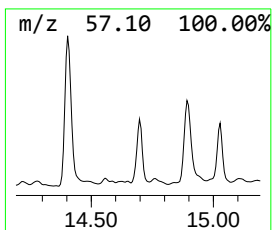
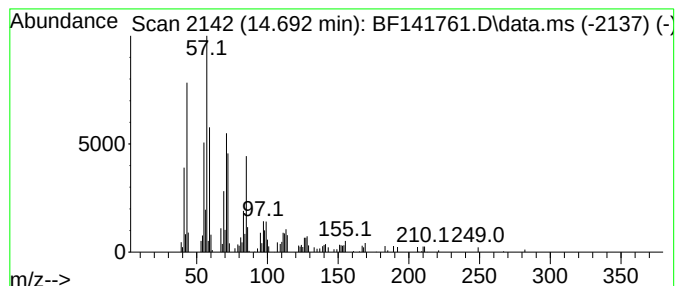
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Eicosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.692	4.34 ng	110028	Perylene-d12	15.386

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Eicosane	282	C20H42	000112-95-8	50
2			Hexacosane	366	C26H54	000630-01-3	46
3			Octadecane, 1-chloro-	288	C18H37Cl	003386-33-2	46
4			Tritetracontane	605	C43H88	007098-21-7	46
5			Tetratetracontane	619	C44H90	007098-22-8	46



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF022525\
Data File : BF141761.D
Acq On : 25 Feb 2025 13:37
Operator : RC/JU
Sample : Q1421-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

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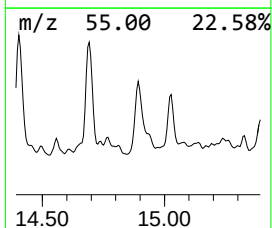
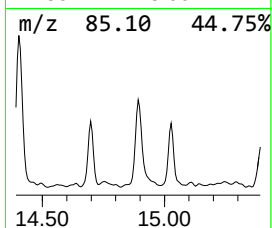
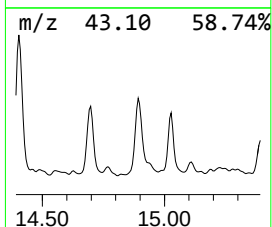
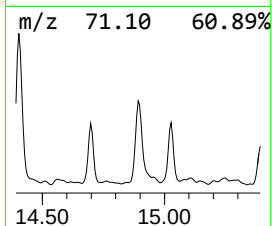
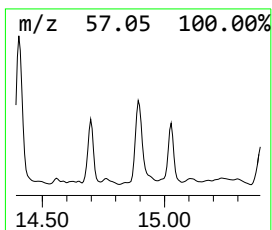
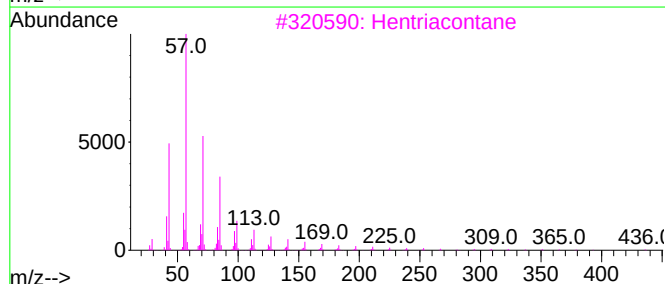
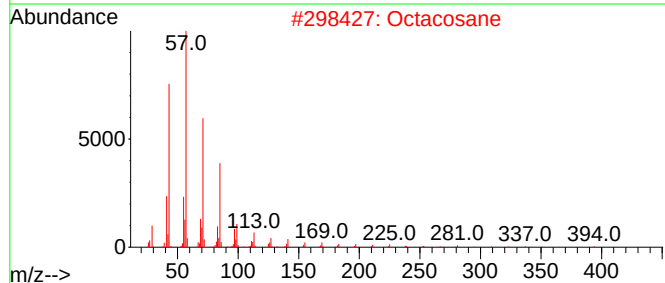
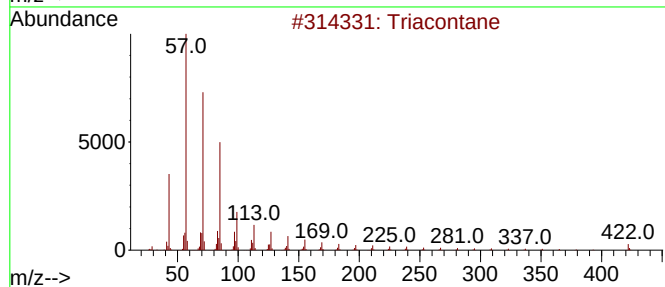
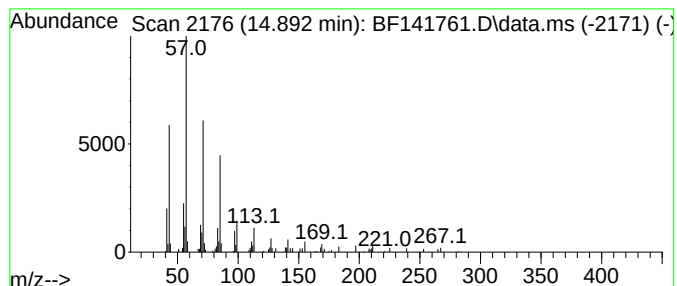
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 Triacontane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.892	4.02 ng	101942	Perylene-d12	15.386

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Triacontane	422	C30H62	000638-68-6	91
2			Octacosane	394	C28H58	000630-02-4	91
3			Hentriacontane	437	C31H64	000630-04-6	91
4			Pentacosane	352	C25H52	000629-99-2	91
5			Eicosane, 10-methyl-	296	C21H44	054833-23-7	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF022525\
Data File : BF141761.D
Acq On : 25 Feb 2025 13:37
Operator : RC/JU
Sample : Q1421-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
P001-CLAY-CF01-01

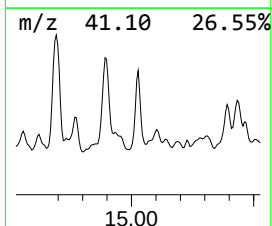
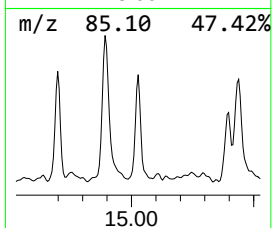
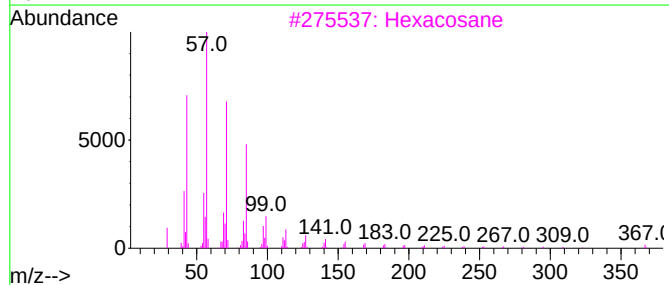
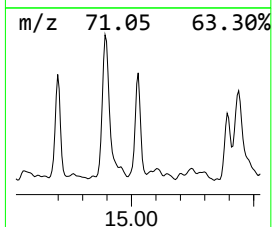
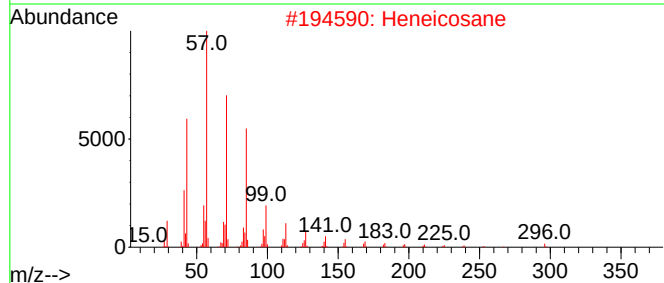
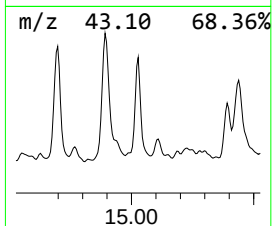
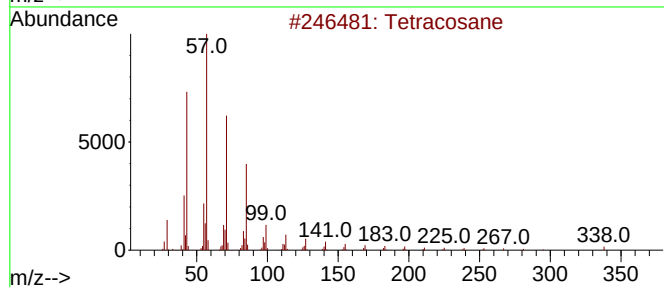
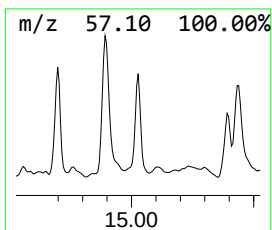
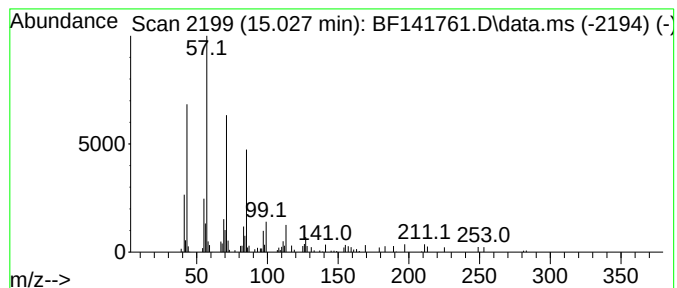
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 14 Tetracosane Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.027	2.55 ng	64722	Perylene-d12	15.386

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetracosane	338	C24H50	000646-31-1	91
2			Heneicosane	296	C21H44	000629-94-7	90
3			Hexacosane	366	C26H54	000630-01-3	90
4			Octacosane	394	C28H58	000630-02-4	90
5			Octacosane, 2-methyl-	408	C29H60	001560-98-1	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF022525\
Data File : BF141761.D
Acq On : 25 Feb 2025 13:37
Operator : RC/JU
Sample : Q1421-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
P001-CLAY-CF01-01

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF020625.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-...	4.987	3.1	ng	66431	1	6.781	424257	20.0
Benzophenone	10.527	8.9	ng	279253	3	9.816	627750	20.0
n-Hexadecanoic ...	11.833	42.0	ng	1253020	4	11.298	596483	20.0
Hentriacontane	12.345	4.3	ng	129227	4	11.298	596483	20.0
13-Octadecenal,...	12.539	2.4	ng	71466	4	11.298	596483	20.0
Octadecanoic acid	12.616	15.4	ng	457712	4	11.298	596483	20.0
1,4-Benzenedica...	12.810	13.5	ng	313863	5	13.939	464226	20.0
Heptacosane	13.239	5.1	ng	119248	5	13.939	464226	20.0
Trichloroacetic...	13.798	4.7	ng	109912	5	13.939	464226	20.0
Hexadecane, 1-i...	13.880	6.7	ng	154879	5	13.939	464226	20.0
Heptadecane, 9-...	14.404	8.4	ng	194181	5	13.939	464226	20.0
Eicosane	14.692	4.3	ng	110028	6	15.386	507231	20.0
Triacontane	14.892	4.0	ng	101942	6	15.386	507231	20.0
Tetracosane	15.027	2.5	ng	64722	6	15.386	507231	20.0