

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102324\
 Data File : BF139982.D
 Acq On : 23 Oct 2024 23:43
 Operator : RC/JU
 Sample : P4385-20
 Misc :
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SP-10

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-BF101824.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF139982.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.205	10	19	26	rVB	1689887	2786409	84.25%	10.281%
2	5.116	506	514	525	rVB	159939	244659	7.40%	0.903%
3	5.504	574	580	586	rBV	2303364	3140172	94.95%	11.586%
4	6.504	744	750	756	rBV	2136808	3051865	92.28%	11.261%
5	6.887	810	815	821	rVB	641707	825276	24.95%	3.045%
6	7.445	904	910	915	rBV	1516765	2016660	60.98%	7.441%
7	7.698	949	953	959	rBV	74495	89396	2.70%	0.330%
8	8.169	1028	1033	1049	rVB	821324	1015555	30.71%	3.747%
9	8.381	1063	1069	1077	rBV	30225	41097	1.24%	0.152%
10	9.245	1210	1216	1226	rBV	2598374	3307121	100.00%	12.202%
11	9.922	1326	1331	1346	rBV	744972	972812	29.42%	3.589%
12	10.634	1447	1452	1459	rBV	130106	165180	4.99%	0.609%
13	10.710	1459	1465	1481	rVV	1231121	1577181	47.69%	5.819%
14	11.410	1579	1584	1592	rBV	685741	908669	27.48%	3.353%
15	11.933	1665	1673	1685	rBV	310680	502757	15.20%	1.855%
16	12.022	1685	1688	1697	rVB2	19270	42934	1.30%	0.158%
17	12.622	1785	1790	1796	rBV	94435	134802	4.08%	0.497%
18	12.722	1802	1807	1814	rBV	63323	110325	3.34%	0.407%
19	12.851	1824	1829	1835	rVB	85640	122033	3.69%	0.450%
20	12.998	1848	1854	1859	rBV	2267990	2927131	88.51%	10.800%
21	13.227	1889	1893	1899	rBV3	18562	44707	1.35%	0.165%
22	13.904	2003	2008	2021	rBV	153358	340801	10.31%	1.257%
23	14.051	2027	2033	2041	rBV	711483	1038194	31.39%	3.831%
24	14.521	2109	2113	2116	rBV	57182	89198	2.70%	0.329%
25	15.092	2207	2210	2219	rVB	52143	107997	3.27%	0.398%
26	15.174	2220	2224	2229	rBV	149504	215070	6.50%	0.794%
27	15.527	2279	2284	2296	rVB	449423	759070	22.95%	2.801%
28	15.768	2321	2325	2331	rBV	82295	135367	4.09%	0.499%
29	16.015	2362	2367	2372	rVB	118618	203072	6.14%	0.749%
30	16.833	2501	2506	2518	rVB	84458	186726	5.65%	0.689%

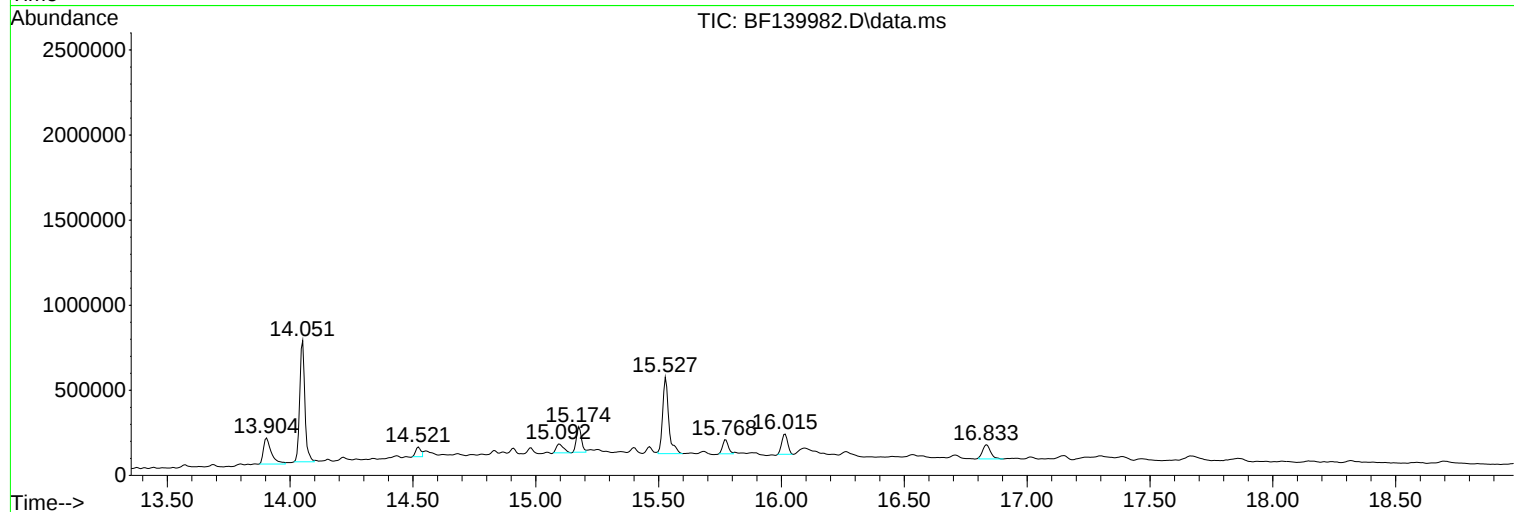
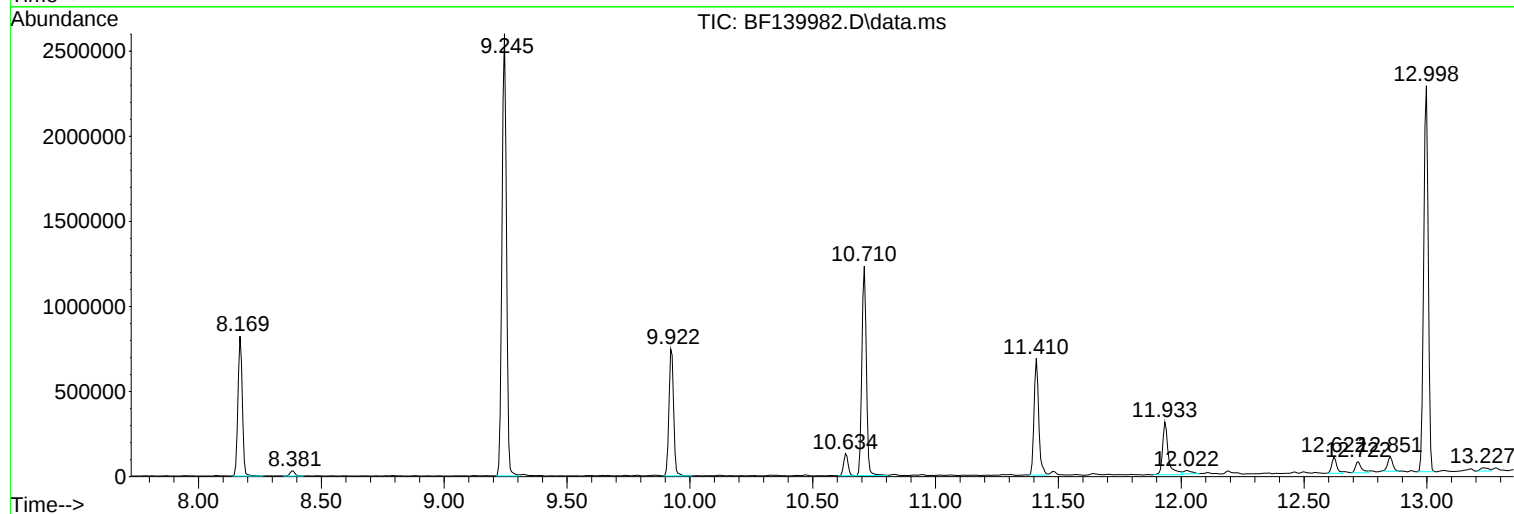
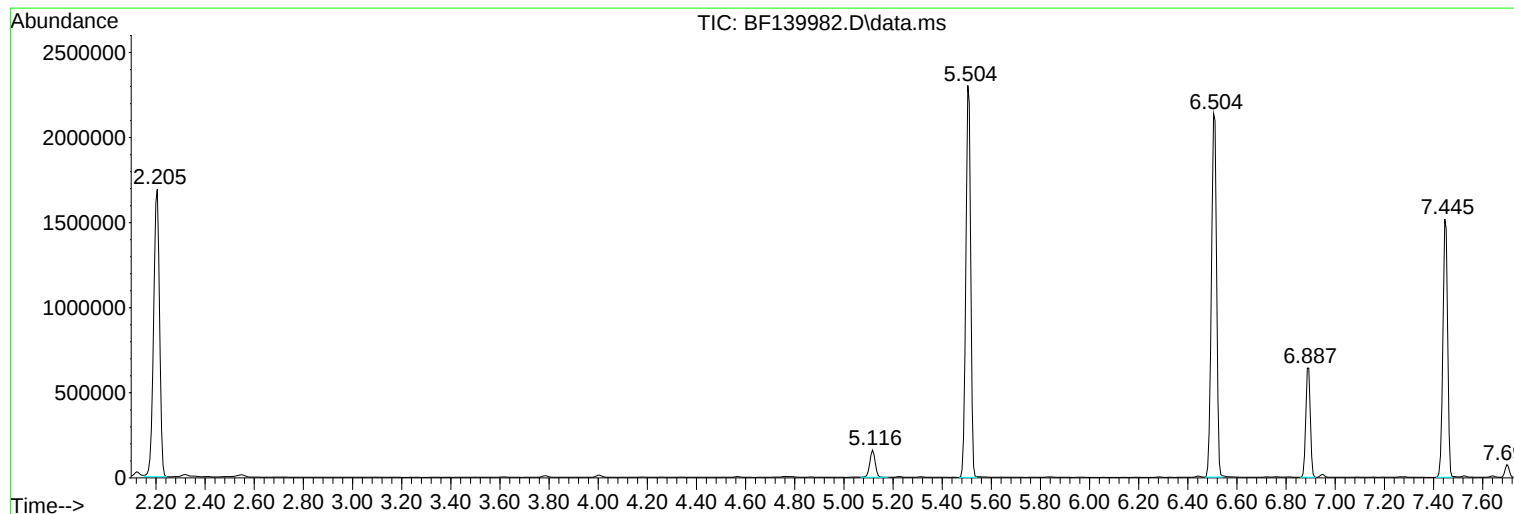
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101824.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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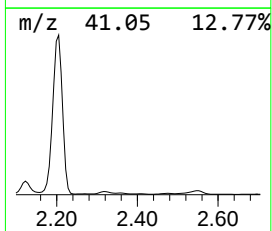
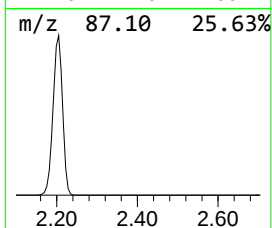
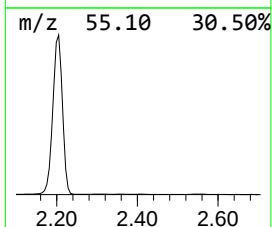
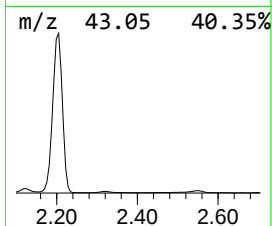
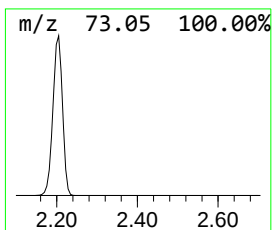
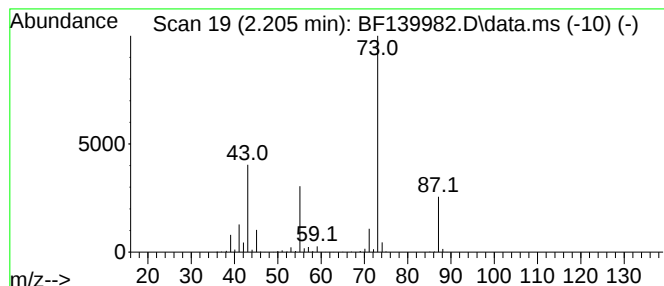
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.205	67.53 ng	2786410	1,4-Dichlorobenzene-d4	6.893

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	39
3			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
4			Octanal, 7-methoxy-3,7-dimethyl-	186	C11H22O2	003613-30-7	17
5			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12



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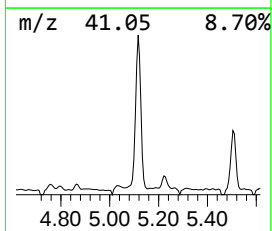
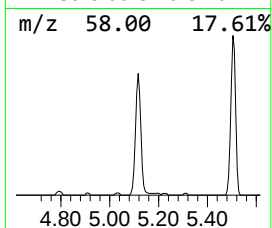
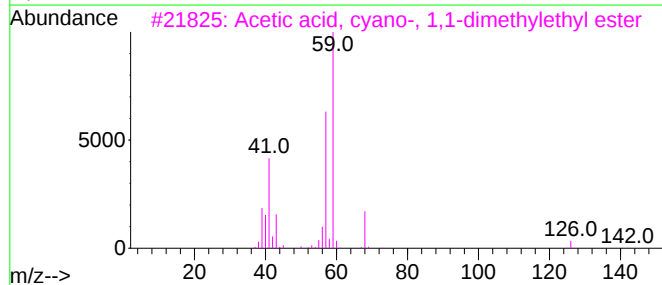
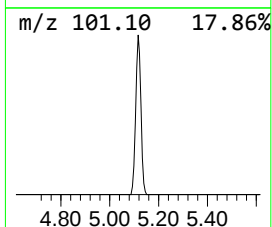
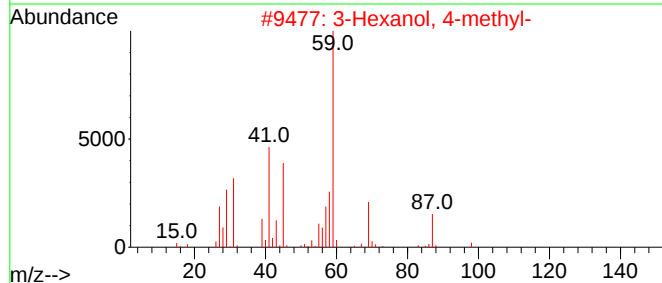
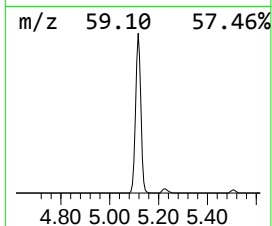
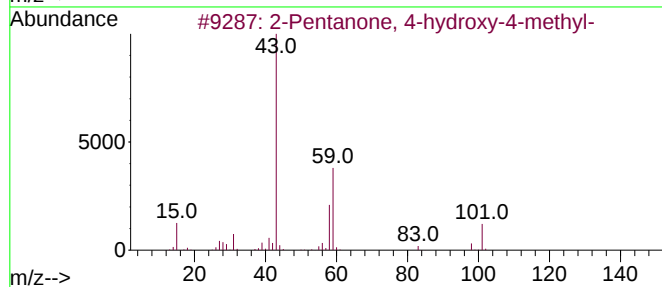
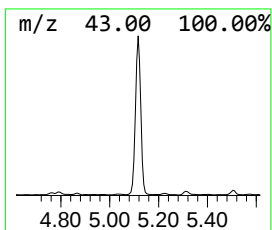
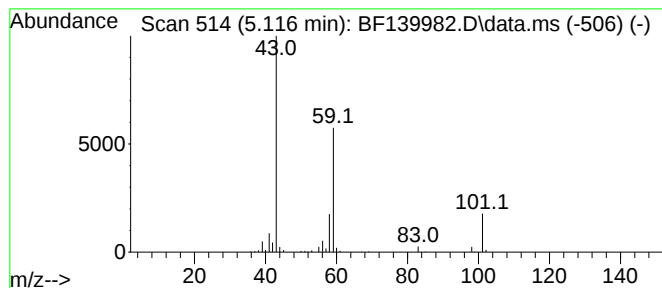
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.116	5.93 ng	244659	1,4-Dichlorobenzene-d4	6.893

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2			3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
3			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
4			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



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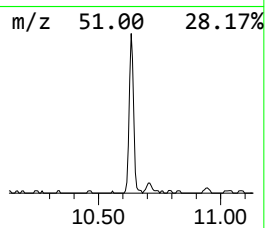
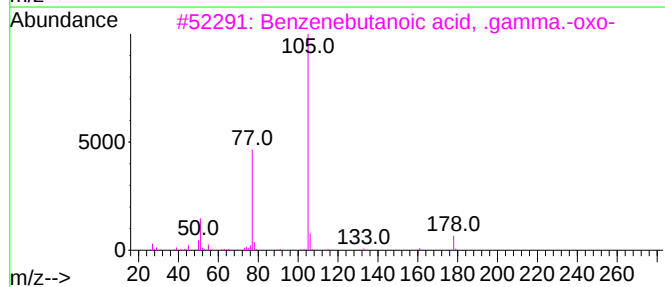
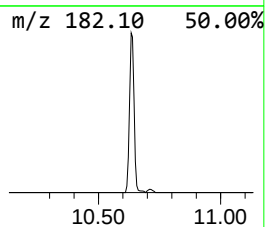
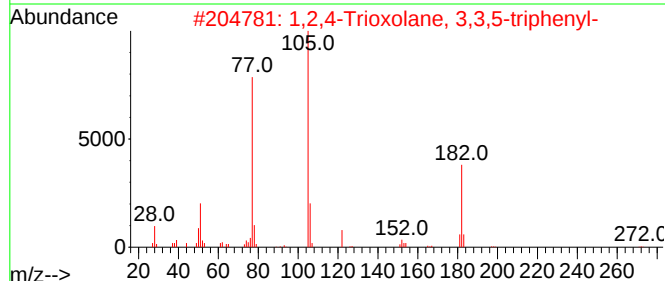
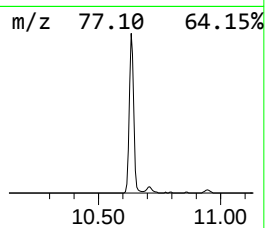
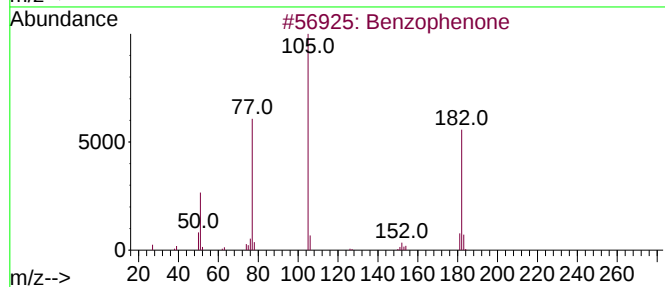
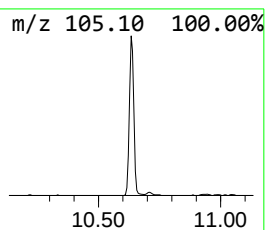
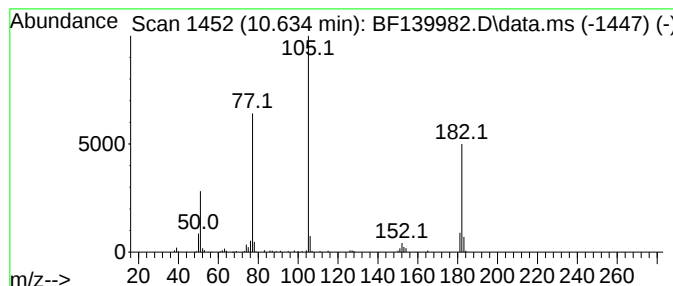
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 Benzophenone Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.634	3.40 ng	165180	Acenaphthene-d10	9.922

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	96
2			1,2,4-Trioxolane, 3,3,5-triphenyl-	304	C20H16O3	023246-12-0	72
3			Benzenebutanoic acid, .gamma.-oxo-	178	C10H10O3	002051-95-8	47
4			1,2-Propanedione, 1-phenyl-	148	C9H8O2	000579-07-7	47
5			N-(1-Cyanovinyl)benzamide	172	C10H8N2O	1000186-19-1	47



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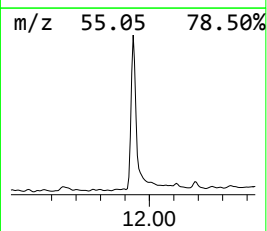
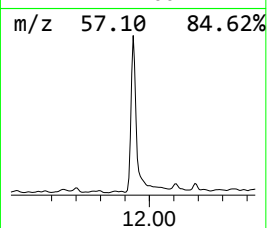
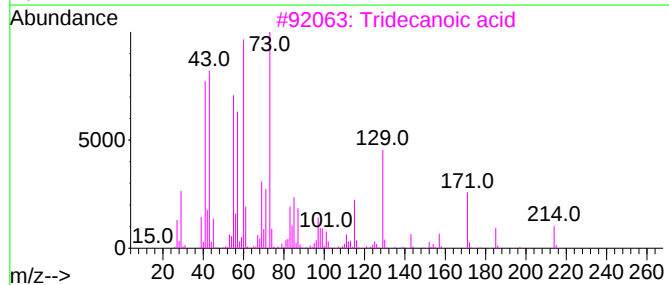
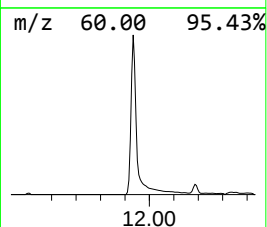
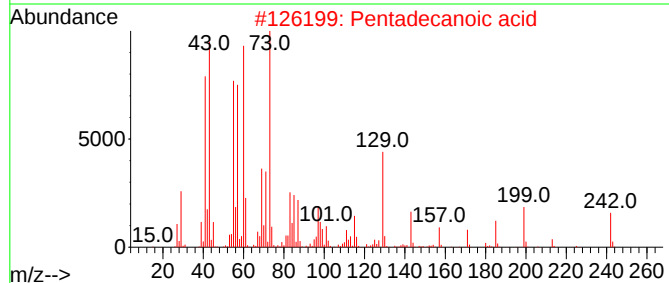
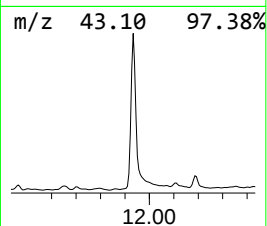
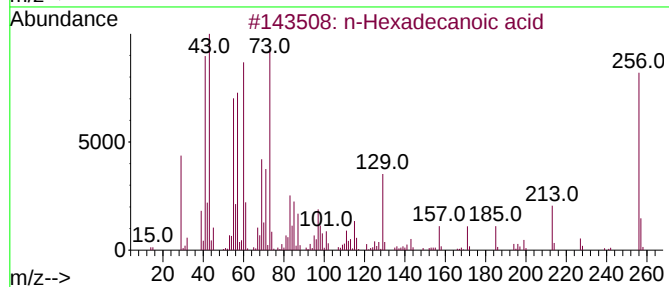
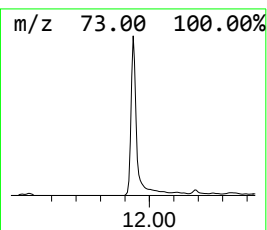
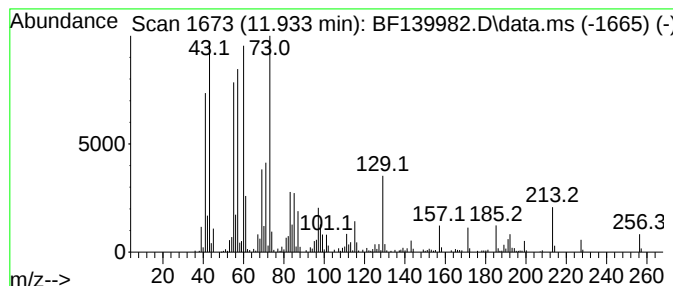
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.933	11.07 ng	502757	Phenanthrene-d10	11.410	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	90
3	Tridecanoic acid	214	C13H26O2	000638-53-9	89
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	68
5	Nonanoic acid	158	C9H18O2	000112-05-0	43



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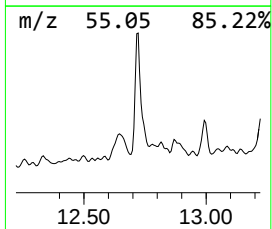
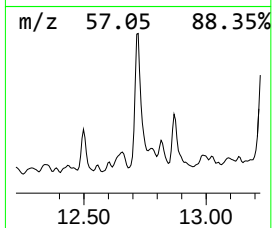
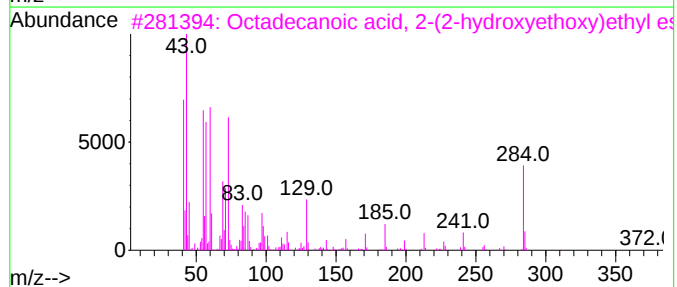
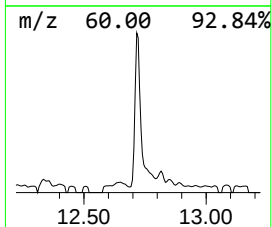
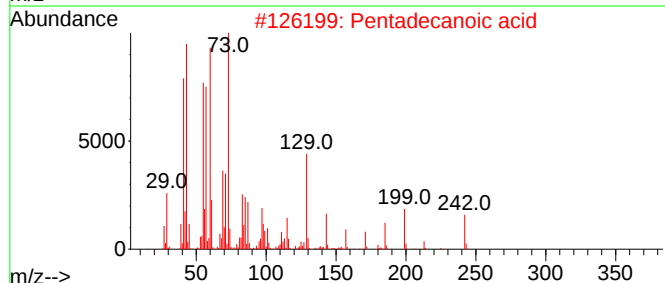
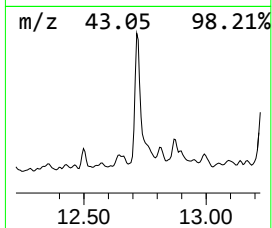
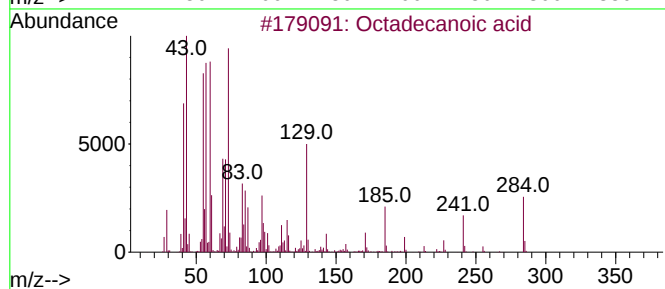
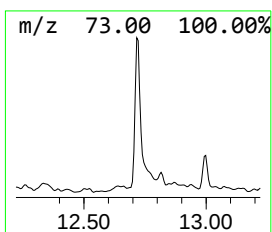
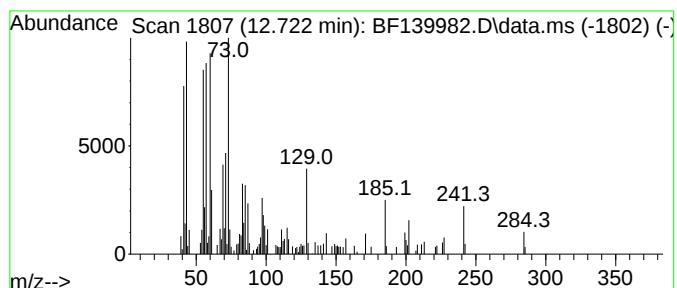
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 Octadecanoic acid Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.722	2.43 ng	110325	Phenanthrene-d10	11.410

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	98
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	95
3			Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	91
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	83
5			Dodecanoic acid	200	C12H24O2	000143-07-7	74



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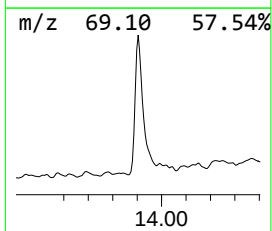
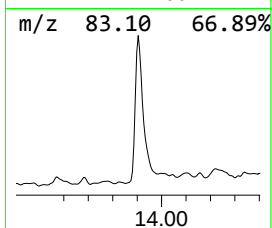
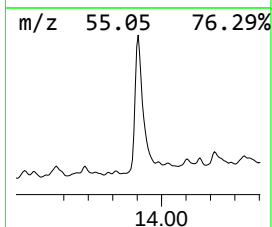
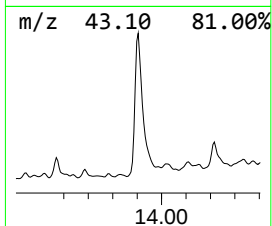
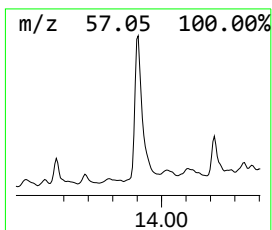
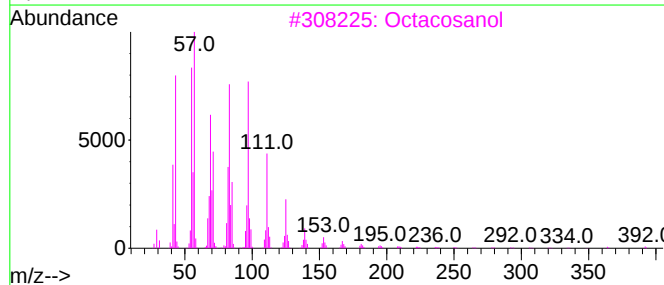
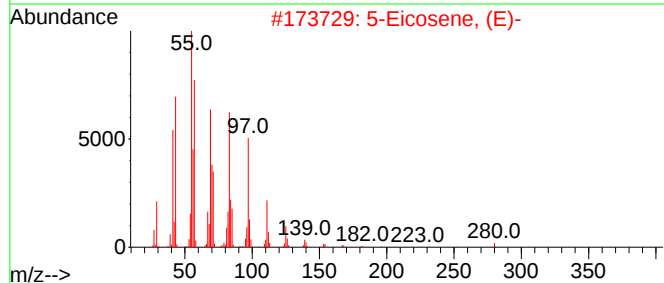
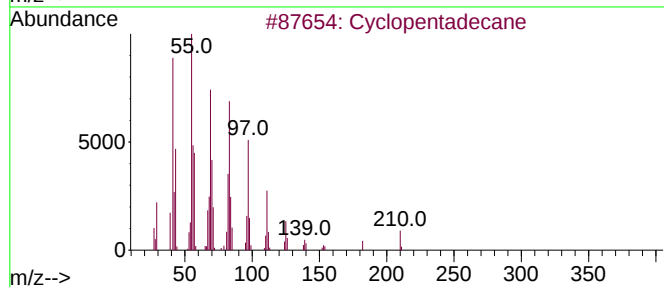
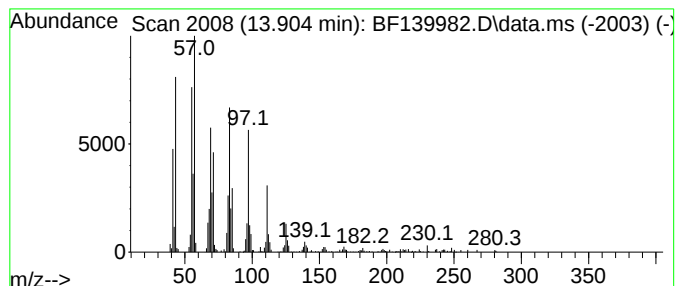
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Cyclopentadecane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.904	6.57 ng	340801	Chrysene-d12	14.051

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopentadecane	210	C15H30	000295-48-7	96
2			5-Eicosene, (E)-	280	C20H40	074685-30-6	95
3			Octacosanol	410	C28H58O	000557-61-9	94
4			Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94
5			1-Hexacosene	364	C26H52	018835-33-1	94



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102324\
Data File : BF139982.D
Acq On : 23 Oct 2024 23:43
Operator : RC/JU
Sample : P4385-20
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SP-10

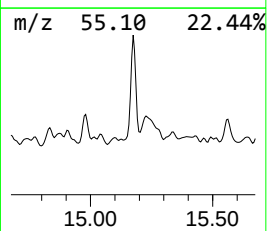
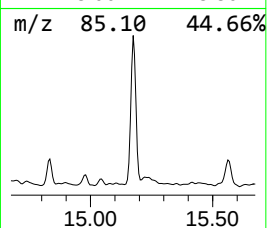
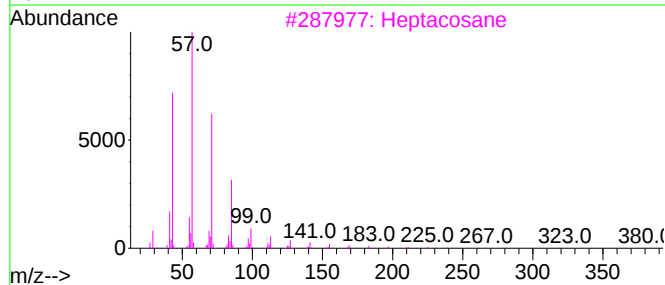
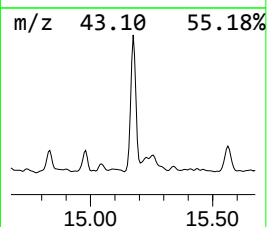
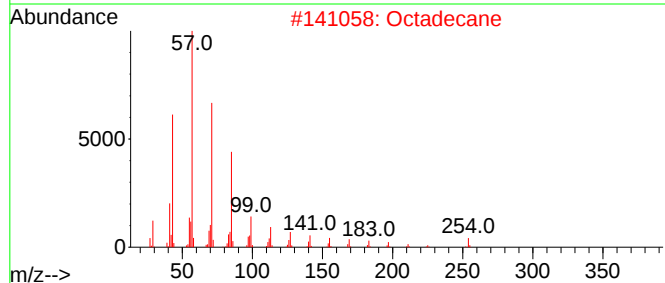
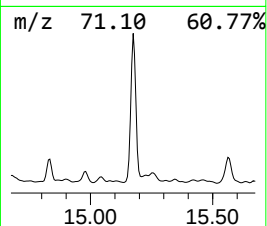
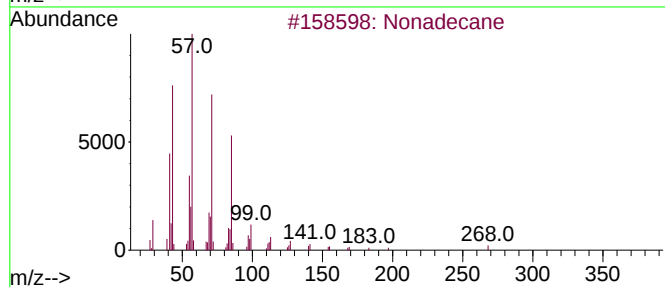
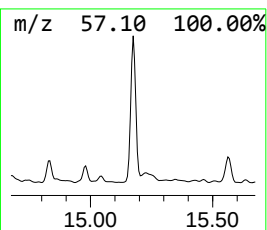
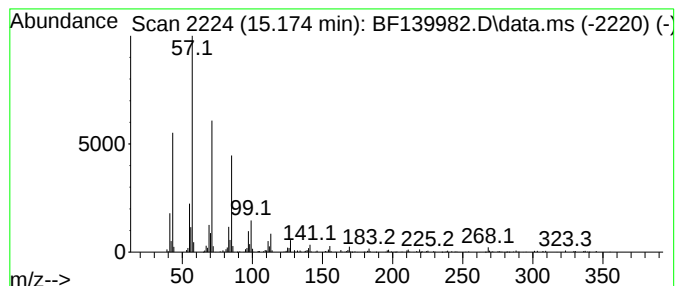
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Nonadecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.174	5.67 ng	215070	Perylene-d12	15.527

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Nonadecane	268	C19H40	000629-92-5	94
2			Octadecane	254	C18H38	000593-45-3	93
3			Heptacosane	380	C27H56	000593-49-7	91
4			Hexacosane	366	C26H54	000630-01-3	91
5			Heneicosane	296	C21H44	000629-94-7	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102324\
Data File : BF139982.D
Acq On : 23 Oct 2024 23:43
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Sample : P4385-20
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SP-10

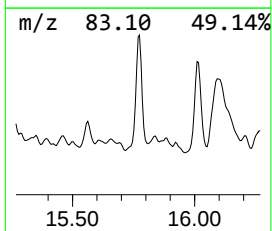
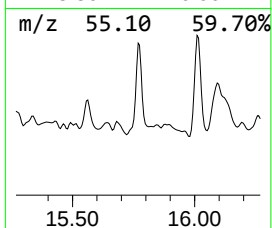
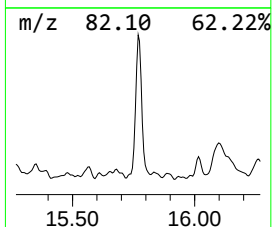
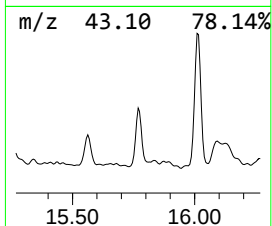
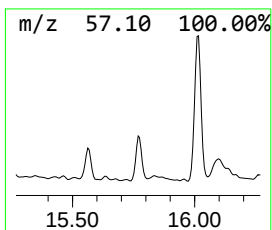
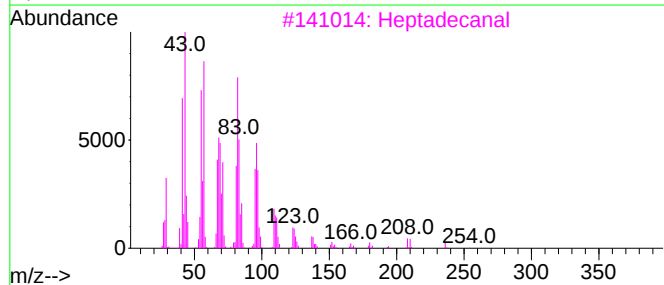
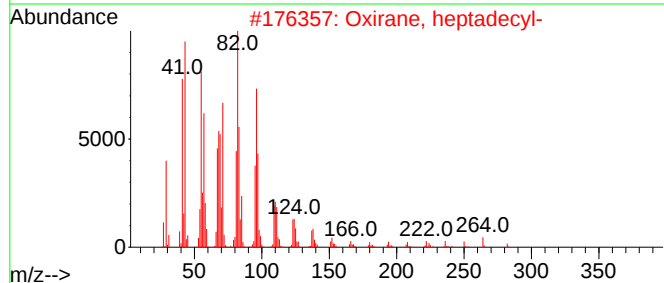
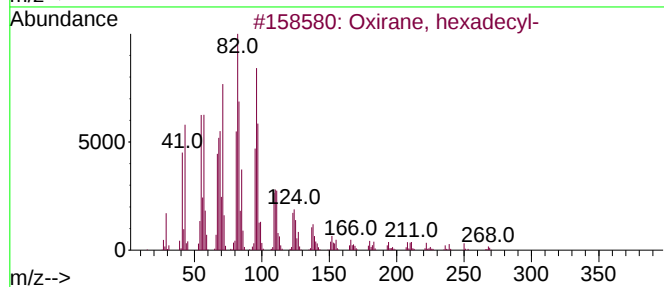
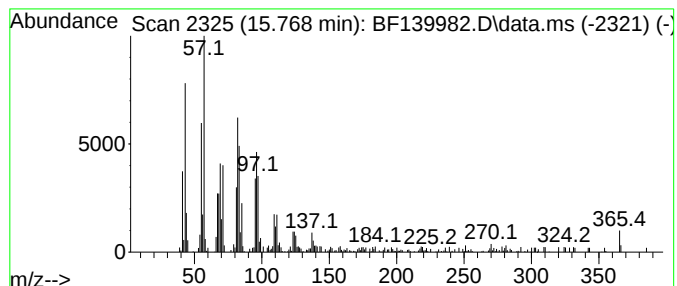
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Oxirane, hexadecyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.769	3.57 ng	135367	Perylene-d12	15.527

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Oxirane, hexadecyl-	268	C18H36O	007390-81-0	93
2			Oxirane, heptadecyl-	282	C19H38O	067860-04-2	93
3			Heptadecanal	254	C17H34O	1000376-70-0	91
4			Hexacosanal	380	C26H52O	026627-85-0	90
5			Eicosanal-	296	C20H40O	002400-66-0	86



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102324\
Data File : BF139982.D
Acq On : 23 Oct 2024 23:43
Operator : RC/JU
Sample : P4385-20
Misc :
ALS Vial : 19 Sample Multiplier: 1

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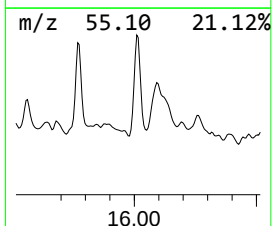
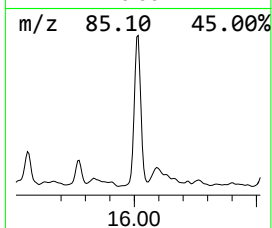
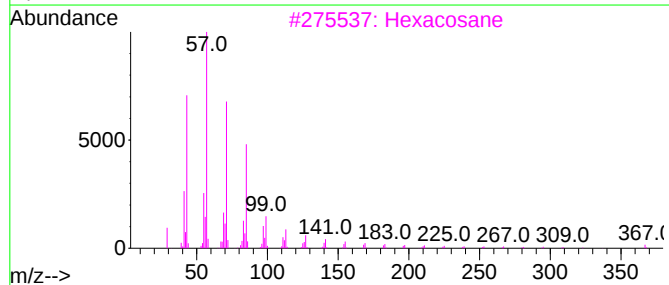
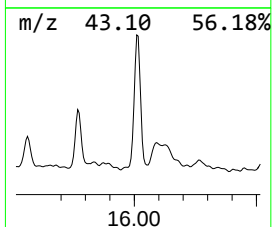
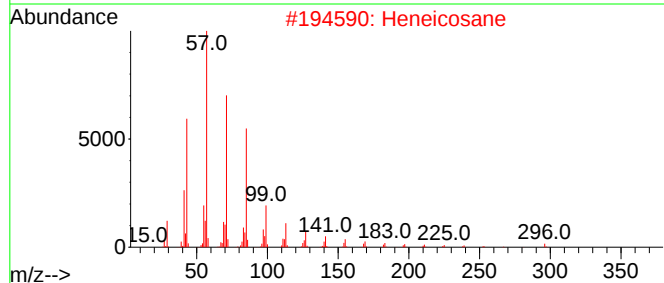
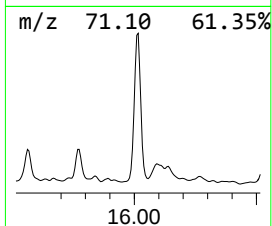
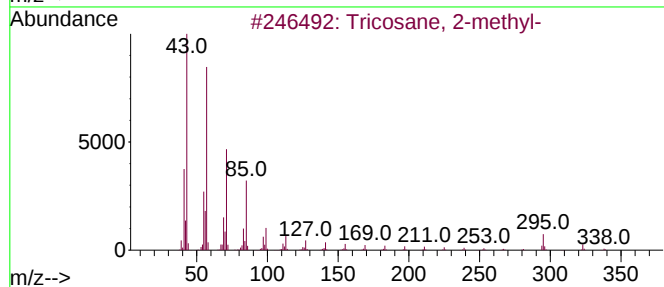
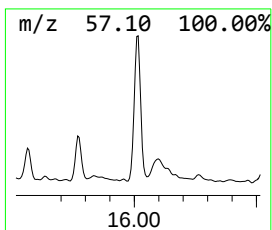
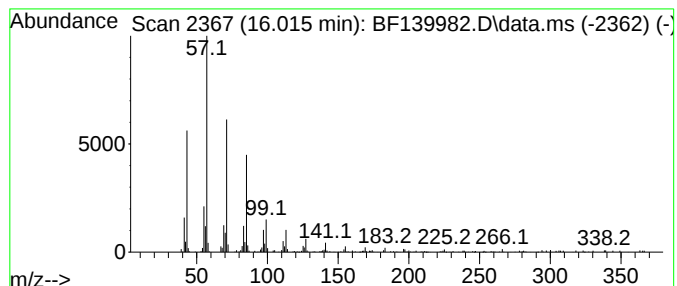
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Tricosane, 2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.015	5.35 ng	203072	Perylene-d12	15.527

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Tricosane, 2-methyl-	338	C24H50	001928-30-9	94
2		Heneicosane	296	C21H44	000629-94-7	91
3		Hexacosane	366	C26H54	000630-01-3	91
4		Dotriacontane, 1-iodo-	576	C32H65I	1000406-32-4	91
5		Octacosane, 2-methyl-	408	C29H60	001560-98-1	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102324\
Data File : BF139982.D
Acq On : 23 Oct 2024 23:43
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Sample : P4385-20
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SP-10

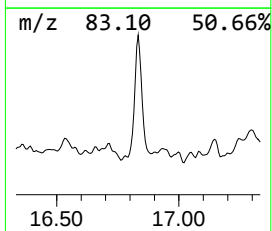
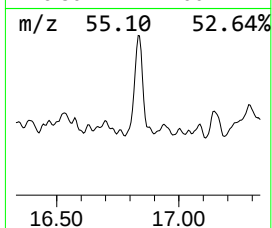
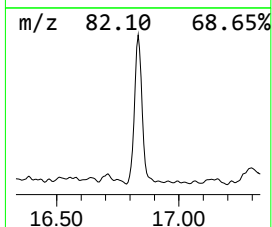
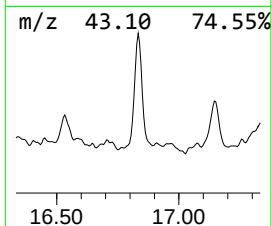
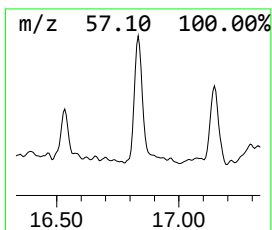
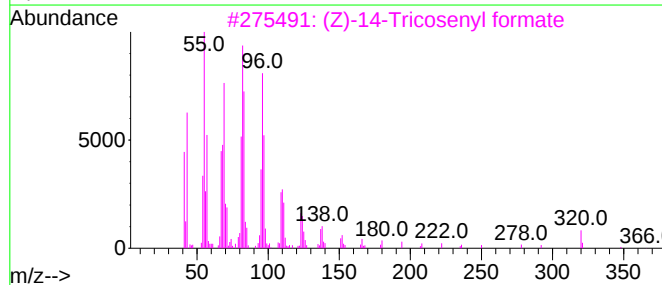
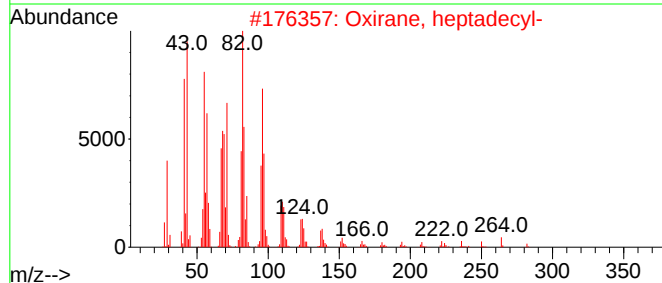
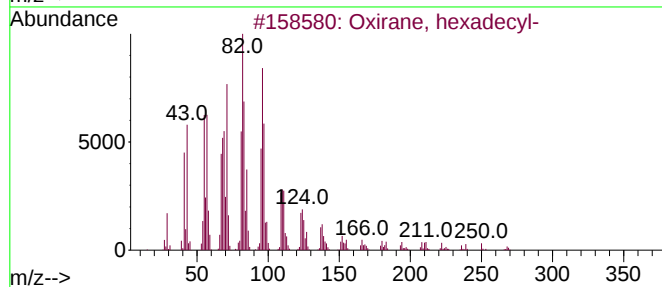
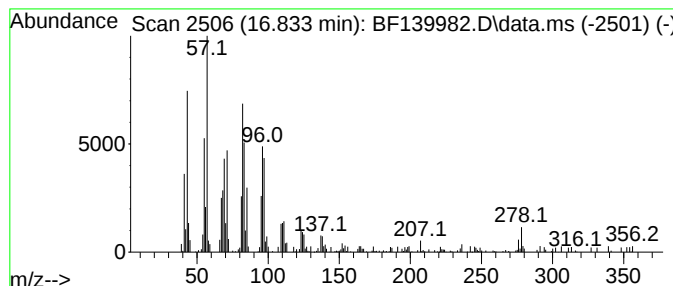
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Oxirane, heptadecyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.833	4.92 ng	186726	Perylene-d12	15.527

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Oxirane, hexadecyl-	268	C18H36O	007390-81-0	87
2		Oxirane, heptadecyl-	282	C19H38O	067860-04-2	62
3		(Z)-14-Tricosenyl formate	366	C24H46O2	077899-10-6	60
4		Tetradecane	198	C14H30	000629-59-4	59
5		Eicosanal-	296	C20H40O	002400-66-0	58



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102324\
Data File : BF139982.D
Acq On : 23 Oct 2024 23:43
Operator : RC/JU
Sample : P4385-20
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101824.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
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2-Pentanone, 4-...	5.116	5.9	ng	244659	1	6.893	825276	20.0
Benzophenone	10.634	3.4	ng	165180	3	9.922	972812	20.0
n-Hexadecanoic ...	11.933	11.1	ng	502757	4	11.410	908669	20.0
Octadecanoic acid	12.722	2.4	ng	110325	4	11.410	908669	20.0
Cyclopentadecane	13.904	6.6	ng	340801	5	14.051	1038190	20.0
Nonadecane	15.174	5.7	ng	215070	6	15.527	759070	20.0
Oxirane, hexade...	15.769	3.6	ng	135367	6	15.527	759070	20.0
Tricosane, 2-me...	16.015	5.3	ng	203072	6	15.527	759070	20.0
Oxirane, heptad...	16.833	4.9	ng	186726	6	15.527	759070	20.0