

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102224\
 Data File : BF139949.D
 Acq On : 23 Oct 2024 01:08
 Operator : RC/JU
 Sample : P4385-10
 Misc :
 ALS Vial : 24 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SP-5

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: BF139949.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.175	6	14	23	rVB	1409349	2286928	90.13%	11.423%
2	5.110	505	513	519	rBV	110792	165713	6.53%	0.828%
3	5.504	574	580	585	rBV	1645496	2108373	83.09%	10.531%
4	6.504	744	750	755	rBV	1506217	1948898	76.81%	9.735%
5	6.893	810	816	821	rVB	530049	656949	25.89%	3.281%
6	7.445	904	910	915	rBV	998477	1253818	49.41%	6.263%
7	7.698	949	953	959	rBV	47198	58011	2.29%	0.290%
8	8.169	1028	1033	1038	rBV	591405	733399	28.90%	3.663%
9	8.387	1064	1070	1076	rBV3	21833	30731	1.21%	0.153%
10	9.245	1210	1216	1226	rBV	1687640	2073429	81.72%	10.357%
11	9.875	1317	1323	1327	rBV	39598	50143	1.98%	0.250%
12	9.928	1327	1332	1336	rVV	573567	736698	29.03%	3.680%
13	9.957	1336	1337	1342	rVB	34567	32844	1.29%	0.164%
14	10.633	1448	1452	1460	rVB	99285	125876	4.96%	0.629%
15	10.710	1460	1465	1475	rBV	990159	1246638	49.13%	6.227%
16	11.410	1579	1584	1592	rBV	648071	837313	33.00%	4.182%
17	11.933	1668	1673	1686	rBV	297155	429101	16.91%	2.143%
18	12.622	1786	1790	1802	rBV	65131	127443	5.02%	0.637%
19	12.722	1802	1807	1814	rBV	47630	84780	3.34%	0.423%
20	12.851	1825	1829	1835	rVB	47473	70328	2.77%	0.351%
21	12.998	1848	1854	1859	rBV	2022195	2537327	100.00%	12.674%
22	13.892	2001	2006	2013	rBV	248487	373370	14.72%	1.865%
23	14.051	2028	2033	2040	rVB	631130	840878	33.14%	4.200%
24	14.521	2110	2113	2119	rVB	70712	95717	3.77%	0.478%
25	15.174	2221	2224	2235	rVB	117899	226162	8.91%	1.130%
26	15.527	2279	2284	2290	rBV	326381	503649	19.85%	2.516%
27	16.015	2362	2367	2372	rBV	143949	243929	9.61%	1.218%
28	16.068	2372	2376	2385	rVB	68073	141969	5.60%	0.709%

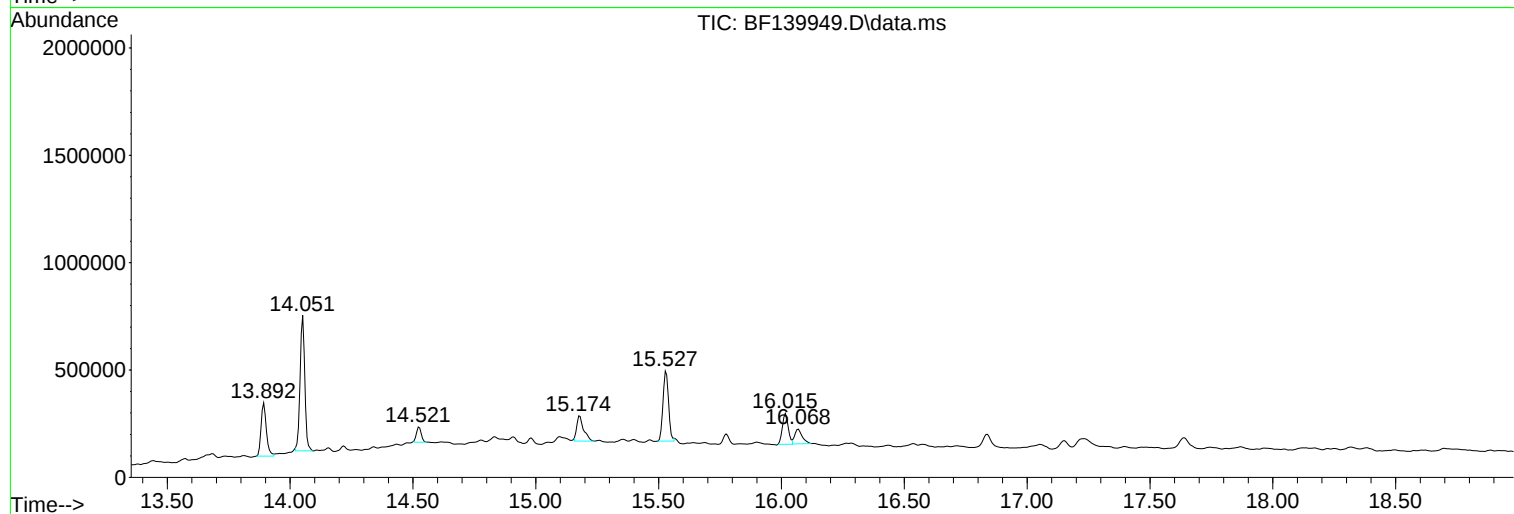
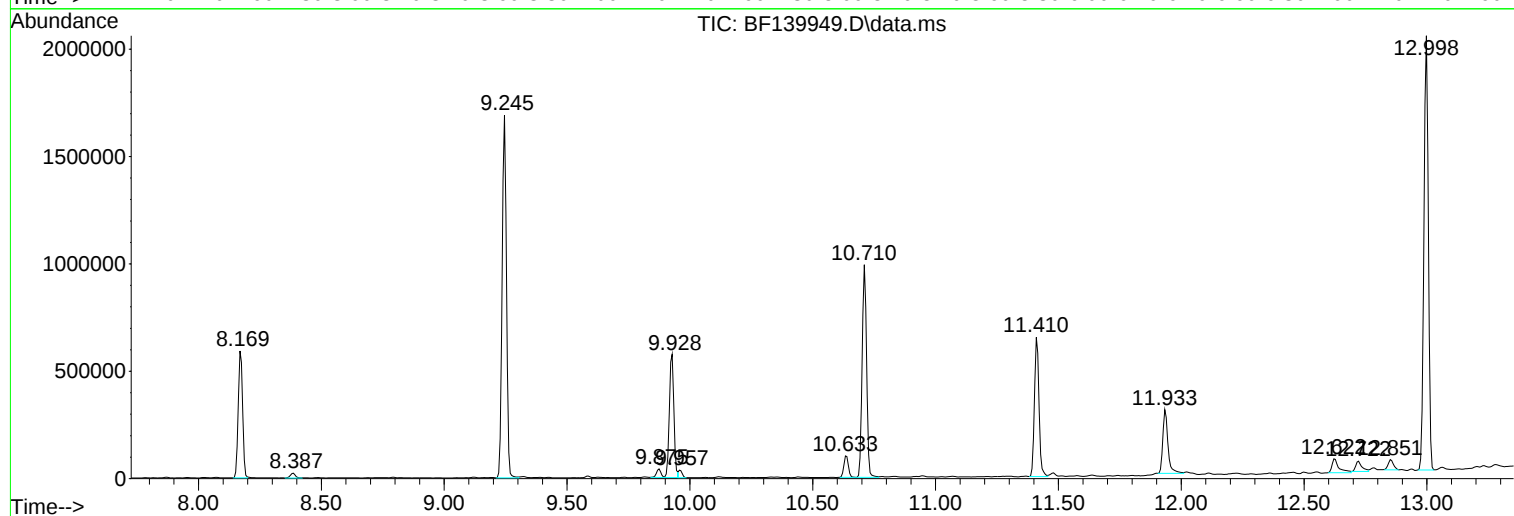
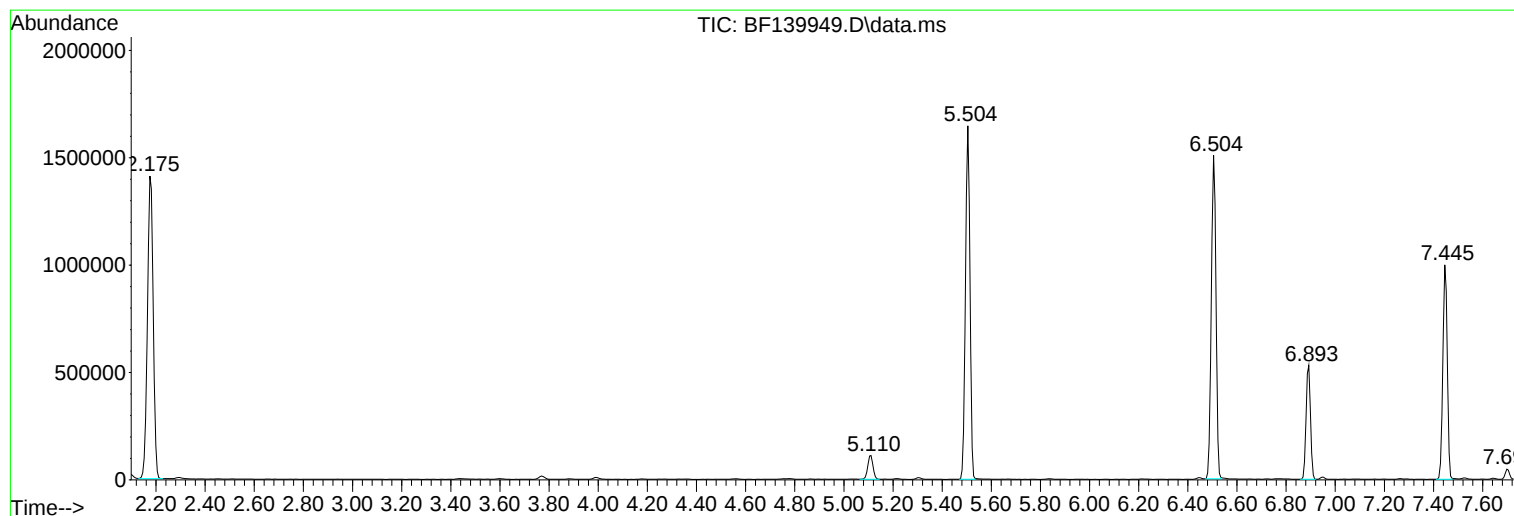
Sum of corrected areas: 20020414

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102224\
Data File : BF139949.D
Acq On : 23 Oct 2024 01:08
Operator : RC/JU
Sample : P4385-10
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SP-5

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



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102224\
Data File : BF139949.D
Acq On : 23 Oct 2024 01:08
Operator : RC/JU
Sample : P4385-10
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SP-5

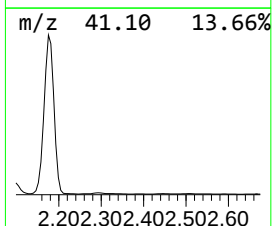
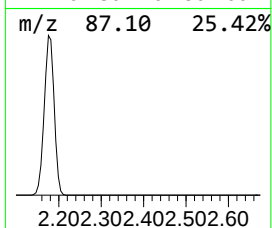
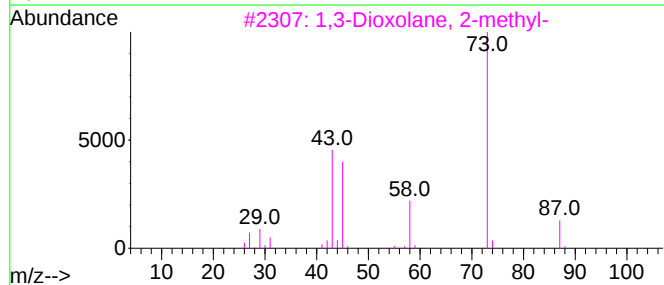
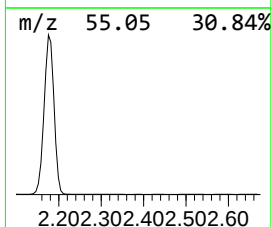
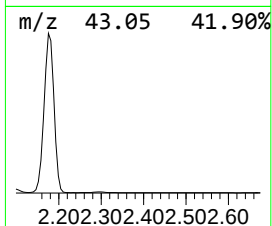
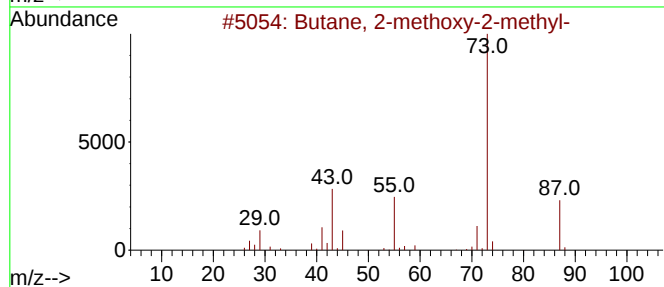
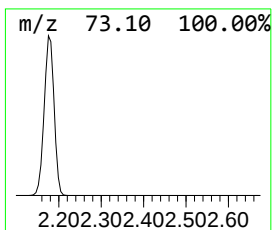
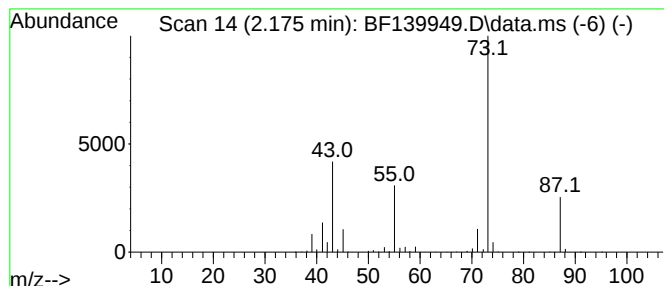
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101824.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.175	69.62 ng	2286930	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	40
3			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	23
4			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12
5			N-Ethylformamide	73	C3H7NO	000627-45-2	9



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102224\
Data File : BF139949.D
Acq On : 23 Oct 2024 01:08
Operator : RC/JU
Sample : P4385-10
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SP-5

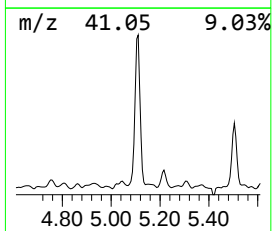
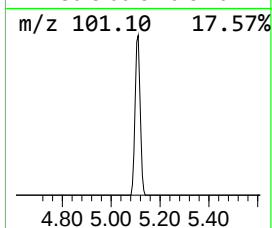
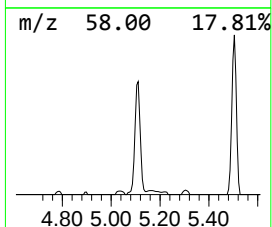
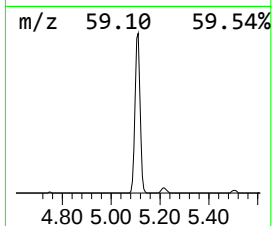
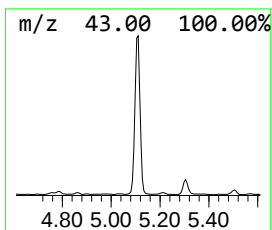
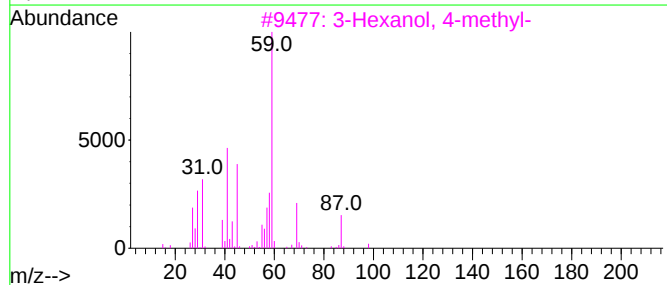
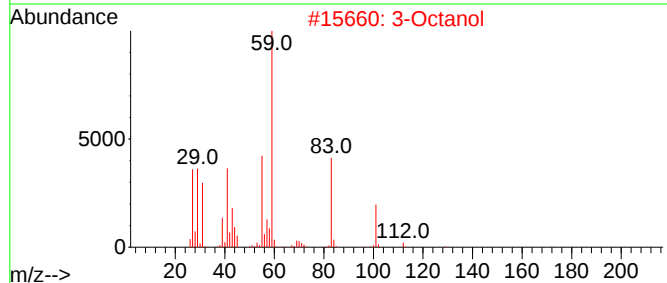
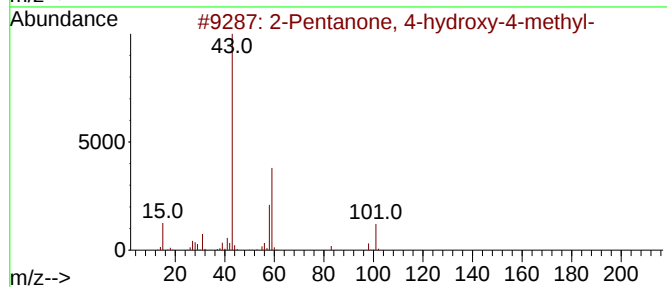
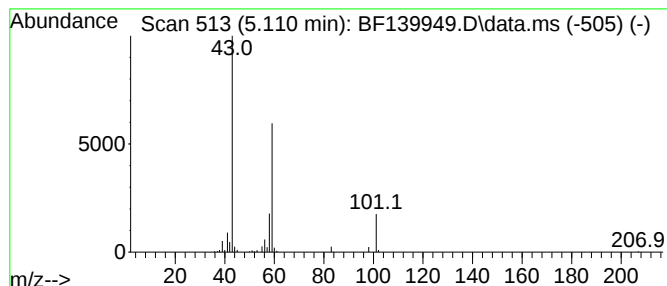
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101824.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.110	5.04 ng	165713	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	50
2		3-Octanol	130	C8H18O	000589-98-0	33
3		3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4		Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	28
5		2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102224\
Data File : BF139949.D
Acq On : 23 Oct 2024 01:08
Operator : RC/JU
Sample : P4385-10
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SP-5

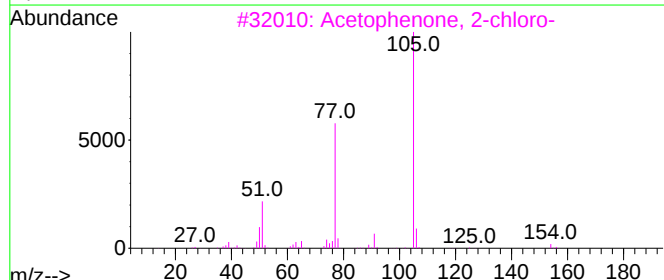
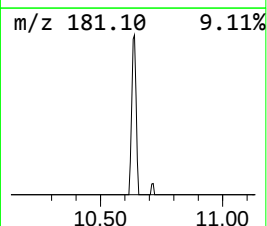
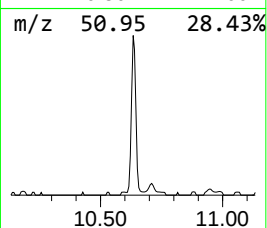
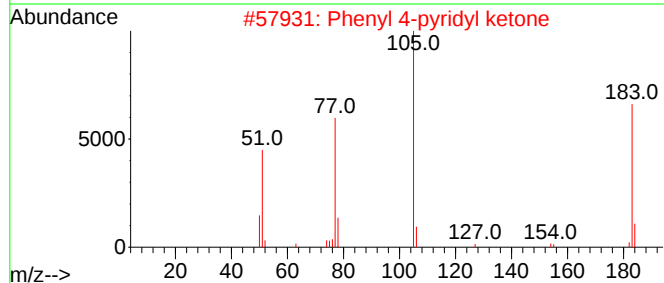
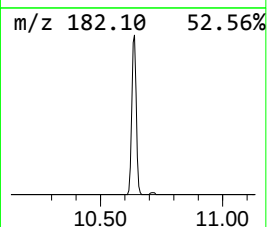
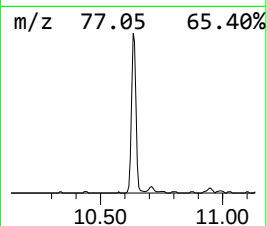
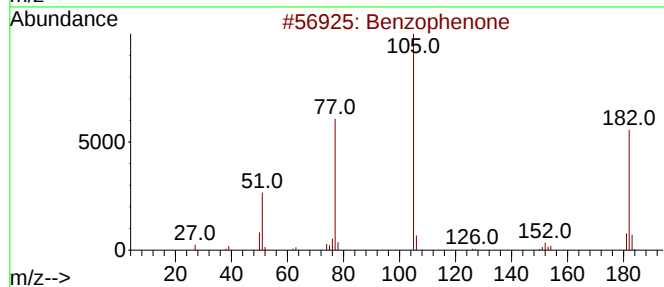
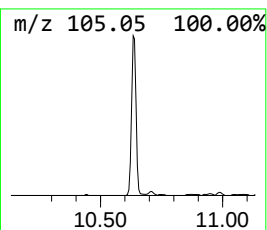
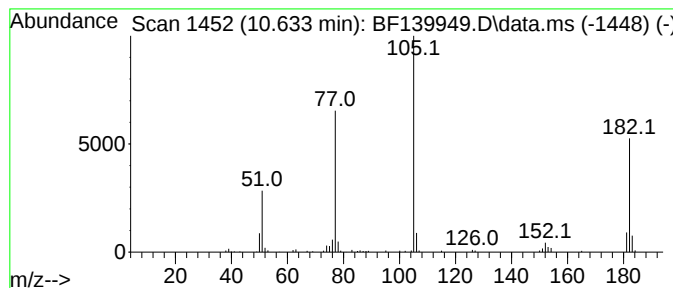
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101824.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 Benzophenone Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.634	3.42 ng	125876	Acenaphthene-d10	9.928

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	96
2			Phenyl 4-pyridyl ketone	183	C12H9NO	014548-46-0	53
3			Acetophenone, 2-chloro-	154	C8H7ClO	000532-27-4	49
4			Benzenecarbothioic acid, S-methy...	152	C8H8OS	005925-68-8	49
5			5-Oxo-5-phenylpentanenitrile	173	C11H11NO	1000486-83-7	47



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102224\
Data File : BF139949.D
Acq On : 23 Oct 2024 01:08
Operator : RC/JU
Sample : P4385-10
Misc :
ALS Vial : 24 Sample Multiplier: 1

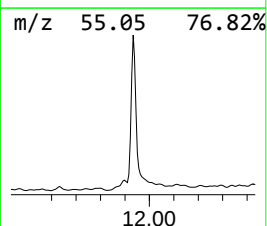
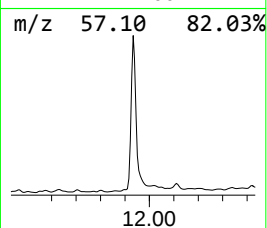
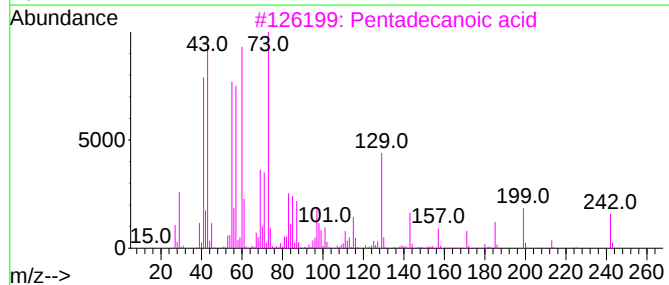
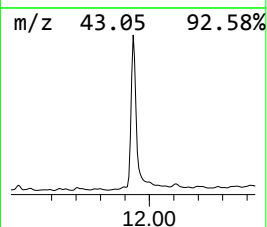
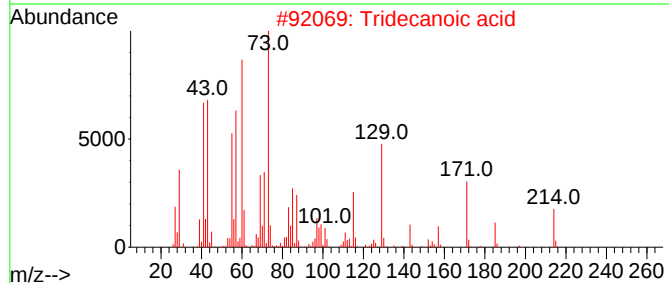
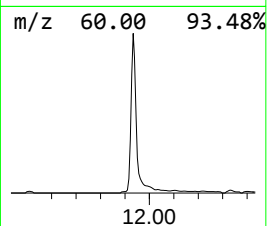
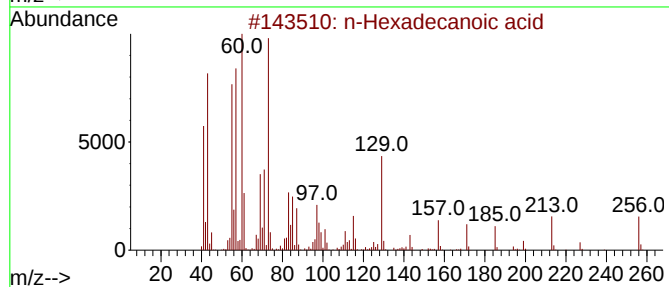
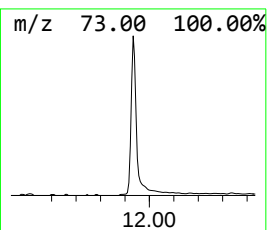
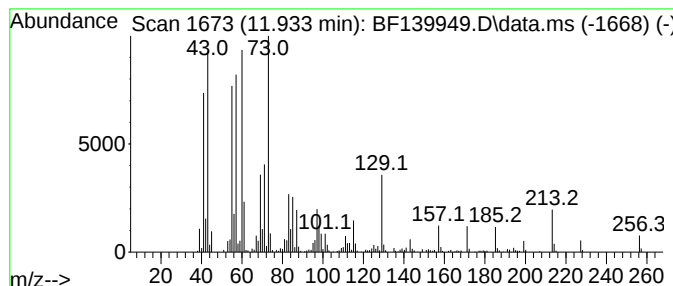
Instrument :
BNA_F
ClientSampleId :
SP-5

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

Peak Number 4 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.933	10.25 ng	429101	Phenanthrene-d10	11.410	
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	93
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	80
5	Carbonic acid, eicosyl vinyl ester	368	C23H44O3	1000382-54-3	35



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102224\
Data File : BF139949.D
Acq On : 23 Oct 2024 01:08
Operator : RC/JU
Sample : P4385-10
Misc :
ALS Vial : 24 Sample Multiplier: 1

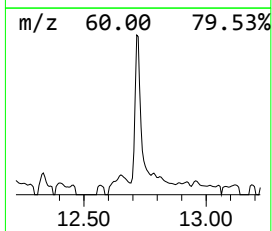
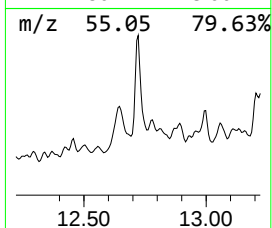
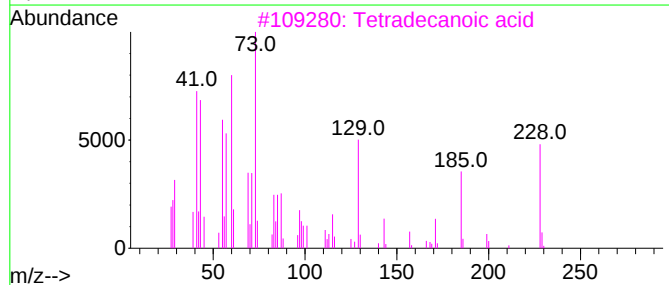
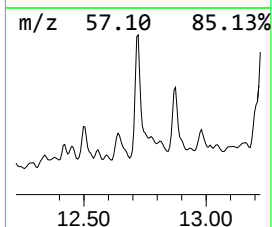
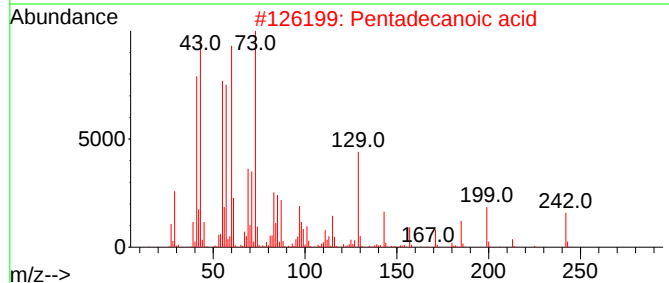
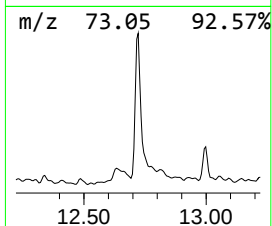
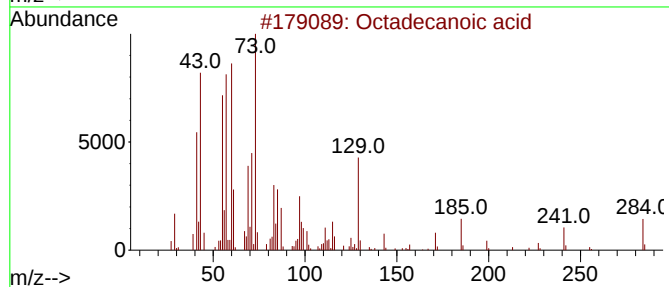
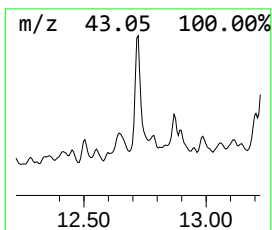
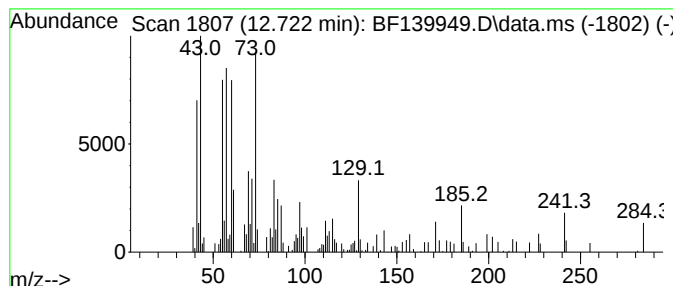
Instrument :
BNA_F
ClientSampleId :
SP-5

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

Peak Number 6 Octadecanoic acid Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.722	2.03 ng	84780	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	97
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	93
4	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	83
5	Tridecanoic acid	214	C13H26O2	000638-53-9	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102224\
Data File : BF139949.D
Acq On : 23 Oct 2024 01:08
Operator : RC/JU
Sample : P4385-10
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SP-5

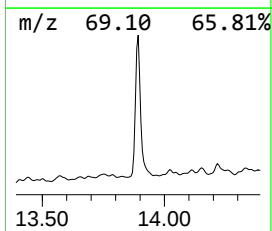
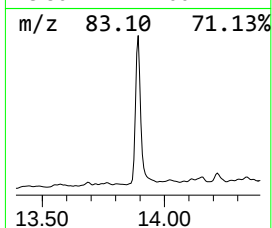
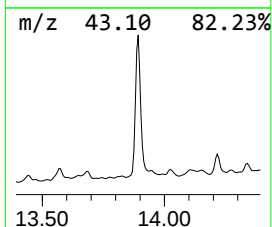
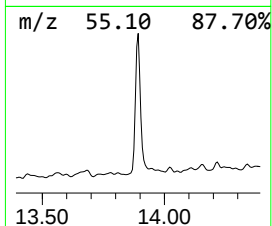
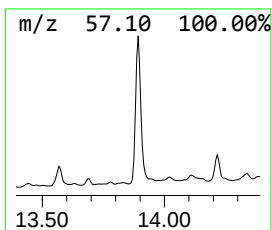
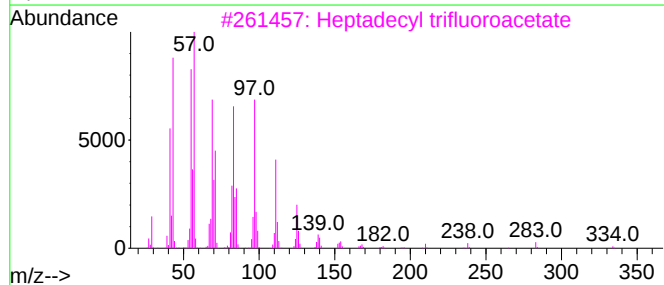
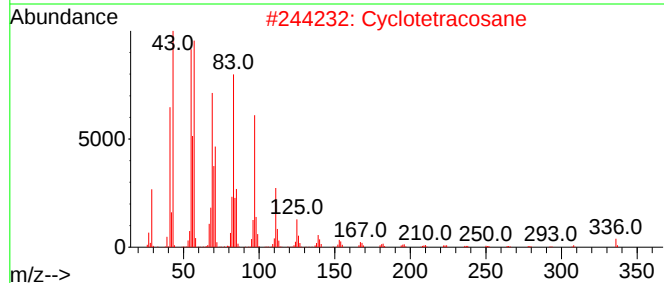
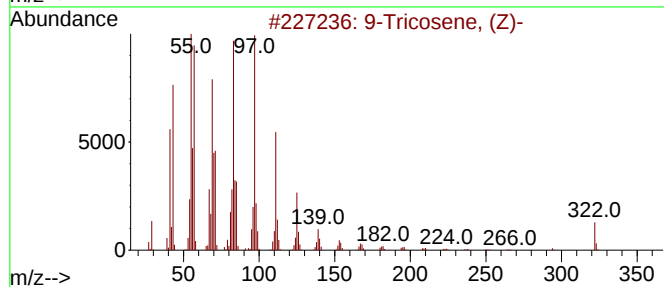
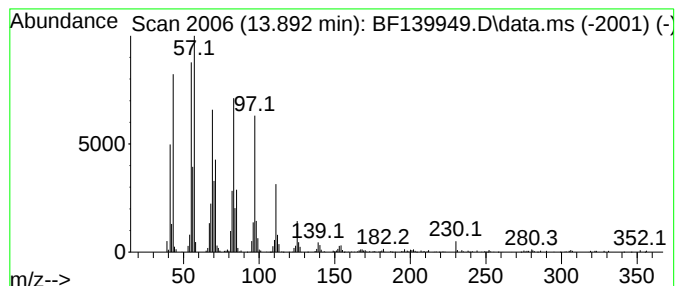
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101824.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 9-Tricosene, (Z)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.892	8.88 ng	373370	Chrysene-d12	14.051

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Tricosene, (Z)-			322	C23H46	027519-02-4	95
2	Cyclotetracosane			336	C24H48	000297-03-0	95
3	Heptadecyl trifluoroacetate			352	C19H35F3O2	1010351-87-0	94
4	Heptafluorobutyric acid, pentade...			424	C19H31F7O2	959261-23-5	94
5	3-Eicosene, (E)-			280	C20H40	074685-33-9	92



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102224\
Data File : BF139949.D
Acq On : 23 Oct 2024 01:08
Operator : RC/JU
Sample : P4385-10
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SP-5

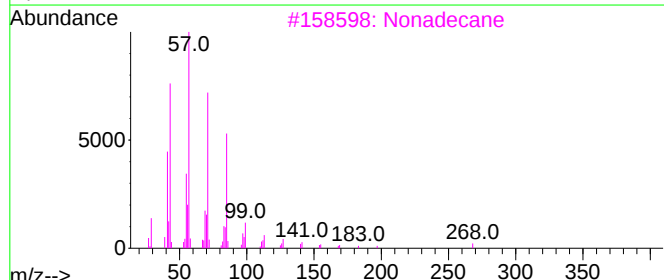
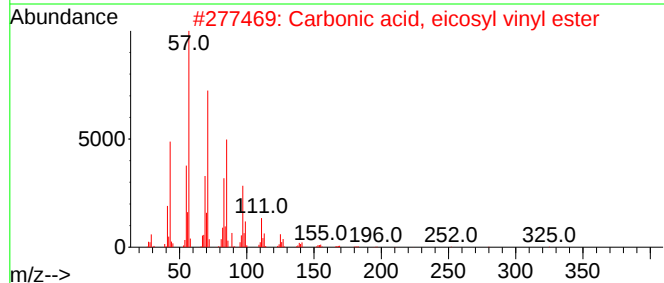
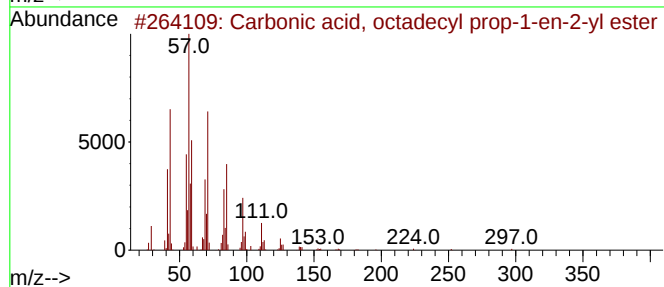
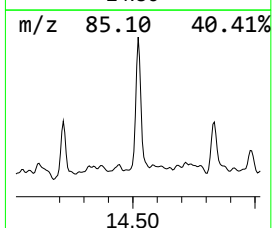
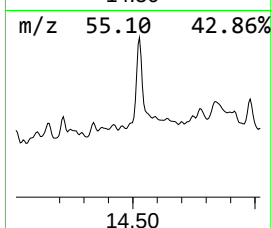
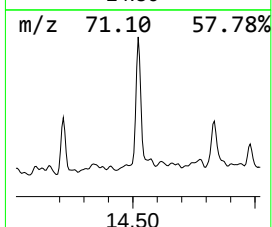
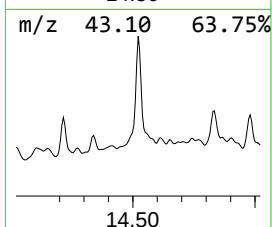
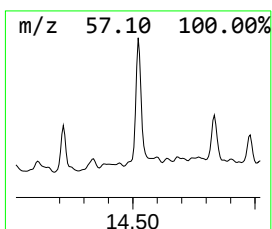
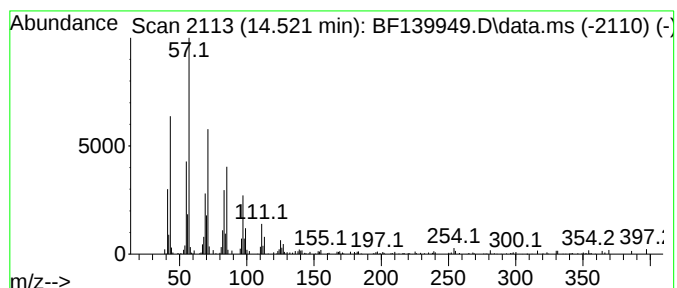
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101824.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Carbonic acid, octadecyl pr... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.522	2.28 ng	95717	Chrysene-d12	14.051

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Carbonic acid, octadecyl prop-1-...	354	C22H42O3	1000383-11-5	94
2			Carbonic acid, eicosyl vinyl ester	368	C23H44O3	1000382-54-3	94
3			Nonadecane	268	C19H40	000629-92-5	93
4			Hexadecane	226	C16H34	000544-76-3	93
5			Octadecane	254	C18H38	000593-45-3	92



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102224\
Data File : BF139949.D
Acq On : 23 Oct 2024 01:08
Operator : RC/JU
Sample : P4385-10
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SP-5

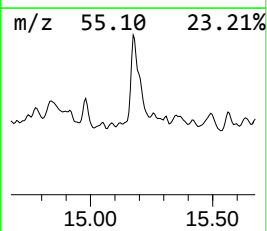
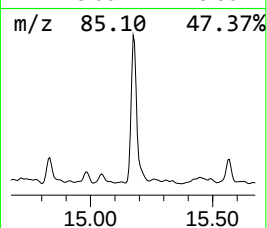
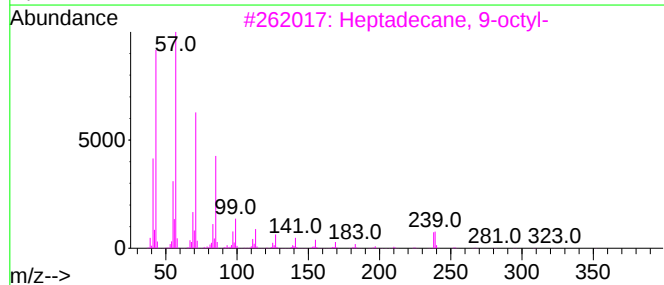
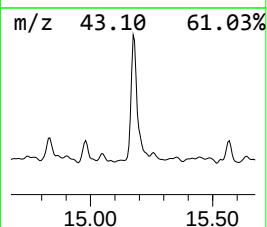
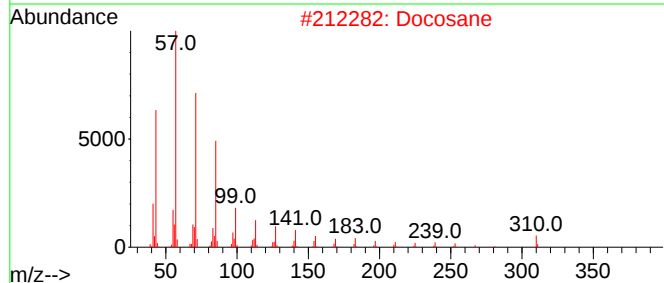
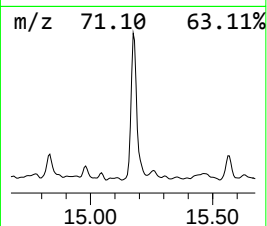
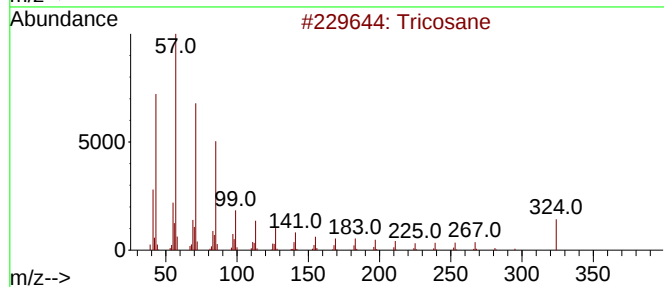
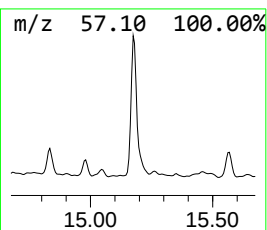
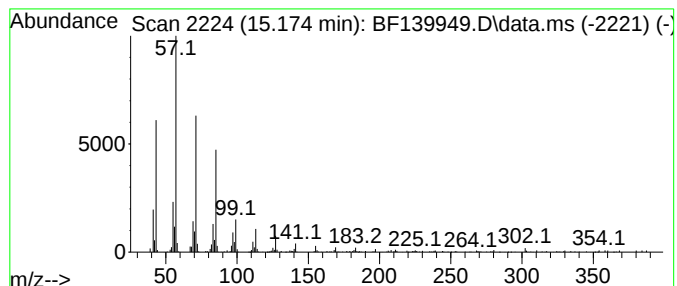
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101824.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Tricosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.174	8.98 ng	226162	Perylene-d12	15.527

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tricosane	324	C23H48	000638-67-5	95
2			Docosane	310	C22H46	000629-97-0	94
3			Heptadecane, 9-octyl-	352	C25H52	007225-64-1	92
4			Octacosane	394	C28H58	000630-02-4	91
5			Heneicosane	296	C21H44	000629-94-7	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102224\
Data File : BF139949.D
Acq On : 23 Oct 2024 01:08
Operator : RC/JU
Sample : P4385-10
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SP-5

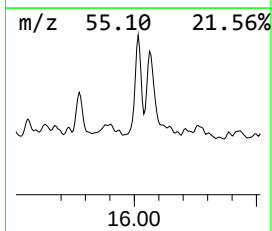
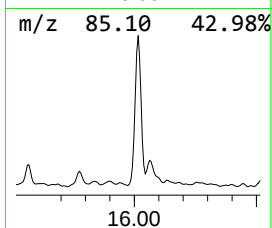
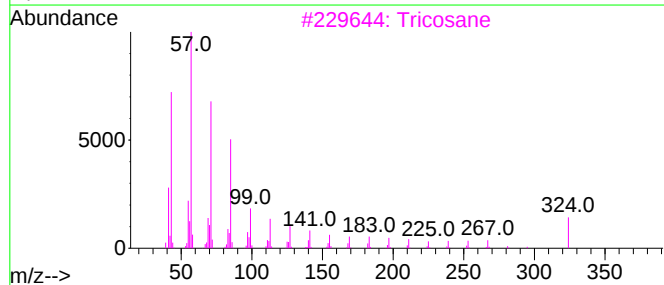
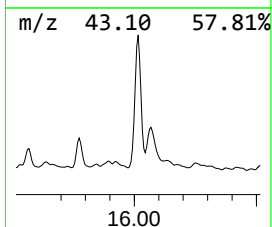
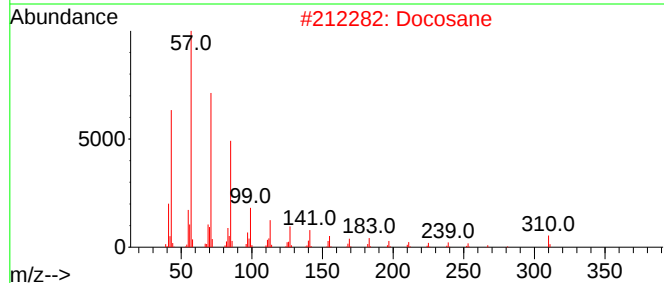
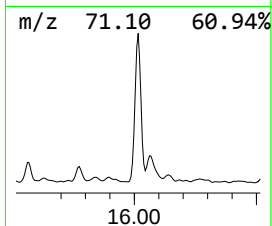
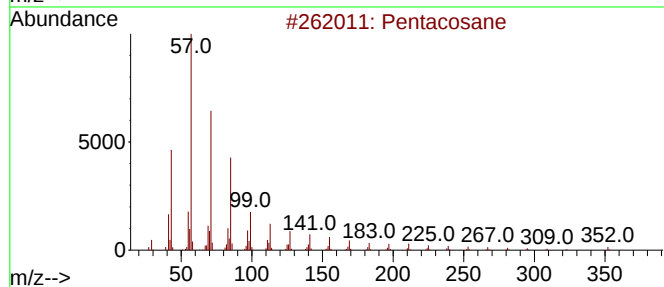
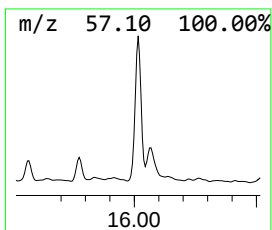
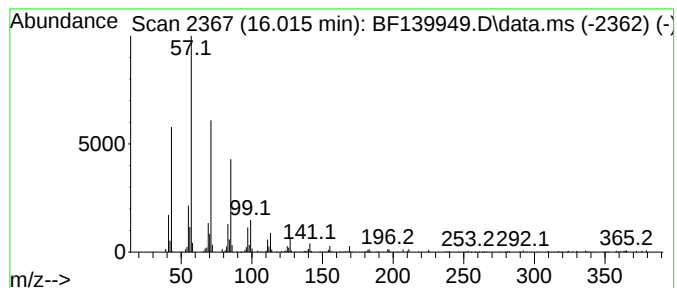
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101824.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Pentacosane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.015	9.69 ng	243929	Perylene-d12	15.527

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentacosane	352	C25H52	000629-99-2	97
2			Docosane	310	C22H46	000629-97-0	96
3			Tricosane	324	C23H48	000638-67-5	94
4			Hexacosane	366	C26H54	000630-01-3	94
5			Docosane, 9-butyl-	366	C26H54	055282-14-9	94



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102224\
Data File : BF139949.D
Acq On : 23 Oct 2024 01:08
Operator : RC/JU
Sample : P4385-10
Misc :
ALS Vial : 24 Sample Multiplier: 1

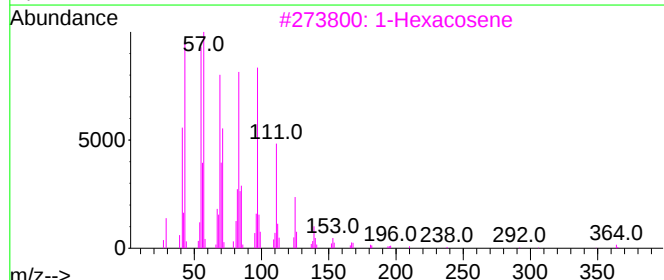
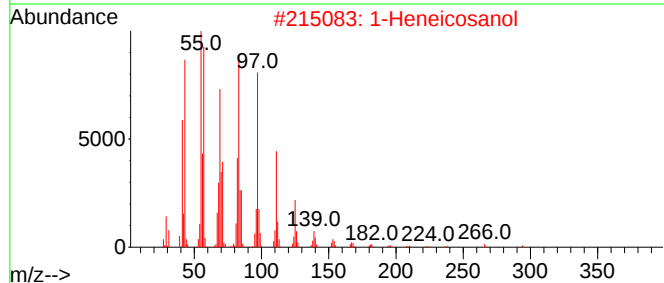
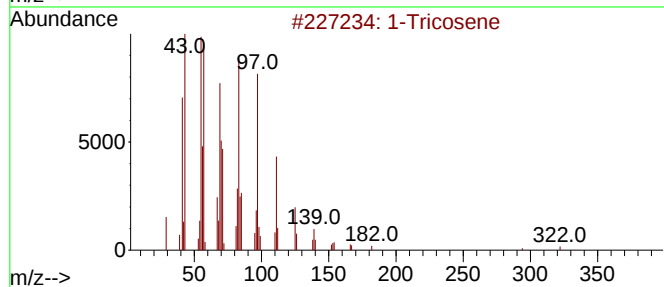
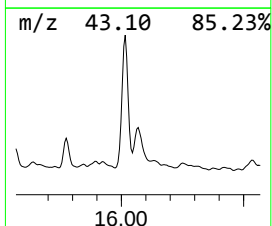
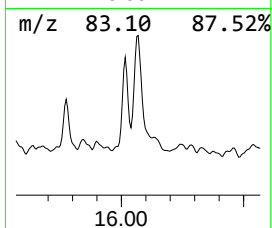
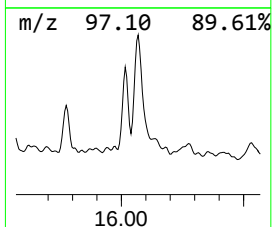
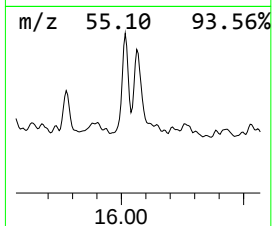
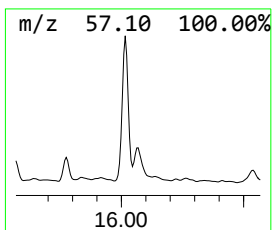
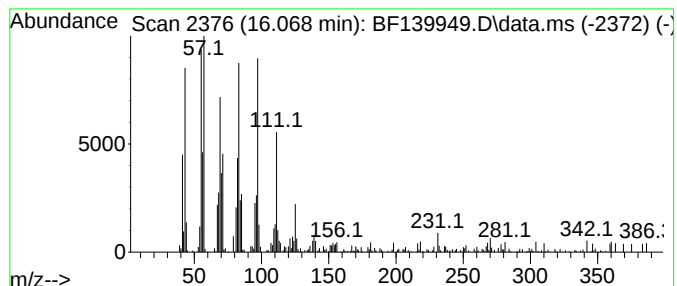
Instrument :
BNA_F
ClientSampleId :
SP-5

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

Peak Number 11 1-Tricosene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
16.068	5.64 ng	141969	Perylene-d12	15.527	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Tricosene	322	C23H46	018835-32-0	99
2	1-Heneicosanol	312	C21H44O	015594-90-8	93
3	1-Hexacosene	364	C26H52	018835-33-1	91
4	1-Heptacosanol	396	C27H56O	002004-39-9	90
5	Octacosyl acetate	452	C30H60O2	018206-97-8	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102224\
Data File : BF139949.D
Acq On : 23 Oct 2024 01:08
Operator : RC/JU
Sample : P4385-10
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SP-5

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
Butane, 2-metho...	2.175	69.6	ng	2286930	1	6.893	656949	20.0
2-Pentanone, 4-...	5.110	5.0	ng	165713	1	6.893	656949	20.0
Benzophenone	10.634	3.4	ng	125876	3	9.928	736698	20.0
n-Hexadecanoic ...	11.933	10.3	ng	429101	4	11.410	837313	20.0
Octadecanoic acid	12.722	2.0	ng	84780	4	11.410	837313	20.0
9-Tricosene, (Z)-	13.892	8.9	ng	373370	5	14.051	840878	20.0
Carbonic acid, ...	14.522	2.3	ng	95717	5	14.051	840878	20.0
Tricosane	15.174	9.0	ng	226162	6	15.527	503649	20.0
Pentacosane	16.015	9.7	ng	243929	6	15.527	503649	20.0
1-Tricosene	16.068	5.6	ng	141969	6	15.527	503649	20.0