

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111524\
 Data File : BF140407.D
 Acq On : 15 Nov 2024 16:47
 Operator : RC/JU
 Sample : P4807-13
 Misc :
 ALS Vial : 18 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TP-6

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-BF111324.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF140407.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.152	3	10	23	rVB	940008	1466988	51.88%	6.998%
2	5.093	498	510	520	rBV	37538	61116	2.16%	0.292%
3	5.504	575	580	597	rBV	1629726	2184717	77.26%	10.422%
4	6.510	745	751	774	rVB	1733363	2385081	84.34%	11.377%
5	6.875	807	813	818	rBV	577030	729934	25.81%	3.482%
6	7.434	902	908	917	rBV	1132976	1499198	53.02%	7.152%
7	7.510	917	921	934	rVB	26375	40599	1.44%	0.194%
8	7.681	945	950	964	rBV	44246	65040	2.30%	0.310%
9	8.151	1025	1030	1048	rVB	715724	942932	33.34%	4.498%
10	9.228	1207	1213	1223	rBV	2194712	2827854	100.00%	13.490%
11	9.910	1323	1329	1343	rVB	816443	1068726	37.79%	5.098%
12	10.622	1445	1450	1458	rBV	164288	205276	7.26%	0.979%
13	10.698	1458	1463	1479	rBV	1230512	1618266	57.23%	7.719%
14	11.398	1577	1582	1590	rBV	889654	1113968	39.39%	5.314%
15	11.463	1590	1593	1599	rVB	25735	31792	1.12%	0.152%
16	11.922	1666	1671	1692	rBV2	114778	215983	7.64%	1.030%
17	12.498	1765	1769	1778	rVB	18395	30140	1.07%	0.144%
18	12.986	1846	1852	1857	rBV	1873244	2468912	87.31%	11.777%
19	13.916	2002	2010	2024	rBV4	29866	127205	4.50%	0.607%
20	14.057	2025	2034	2043	rVB	520005	740181	26.17%	3.531%
21	14.839	2162	2167	2176	rBV	249299	404166	14.29%	1.928%
22	15.574	2286	2292	2305	rVB	444881	735293	26.00%	3.508%

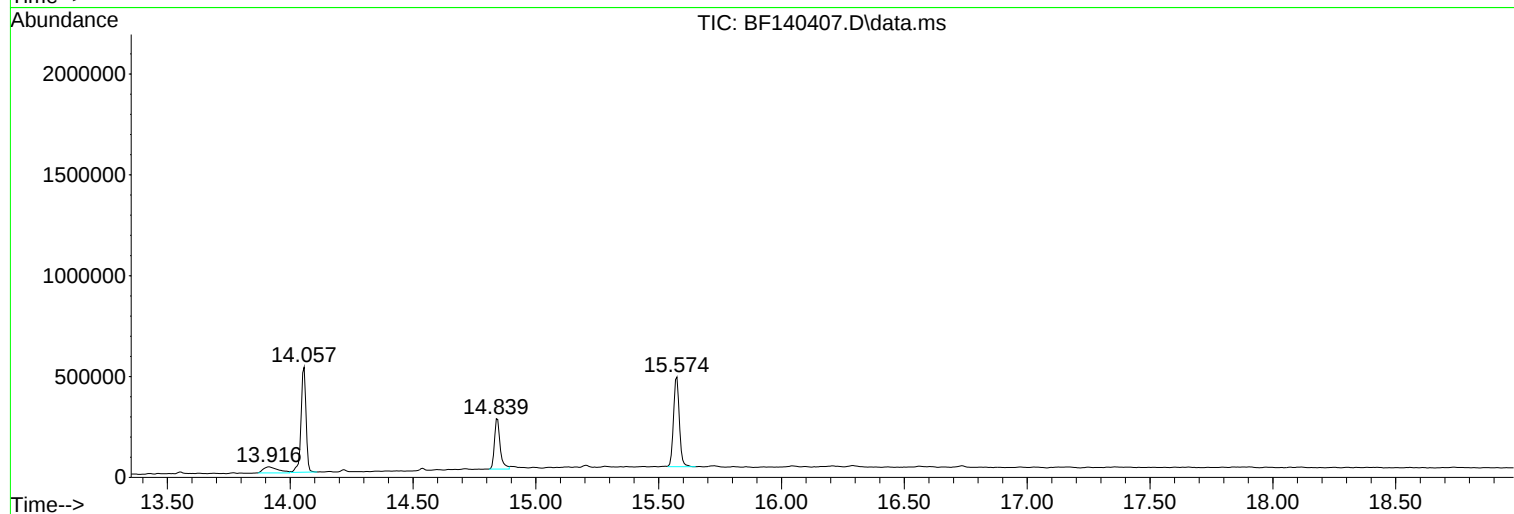
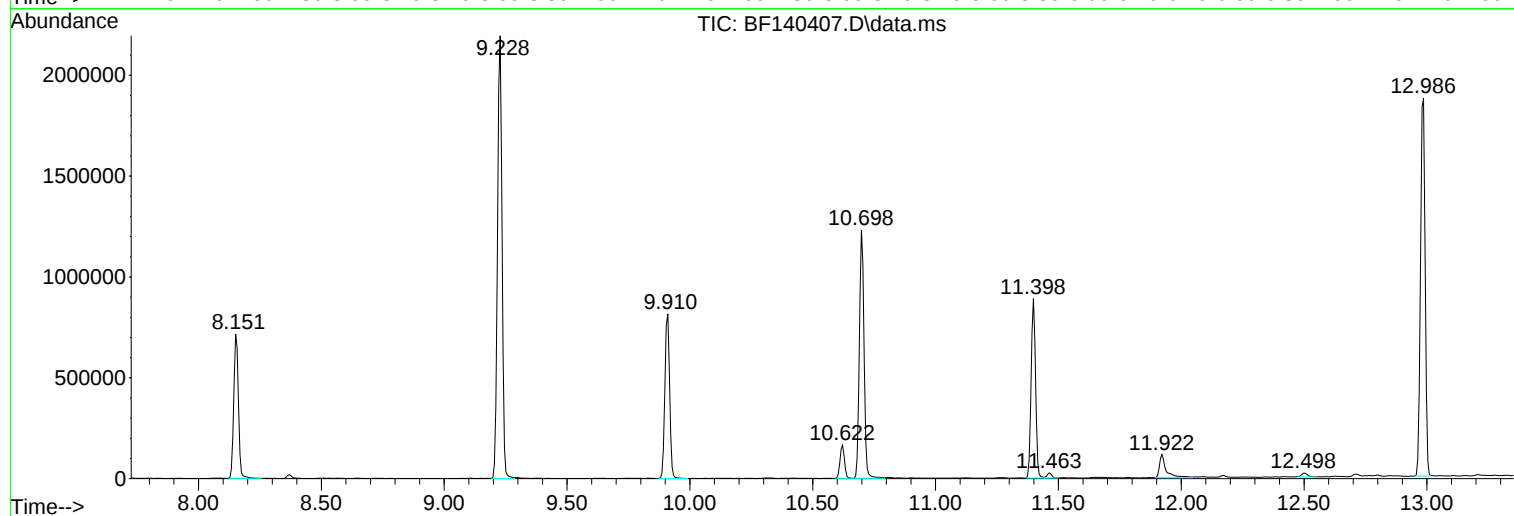
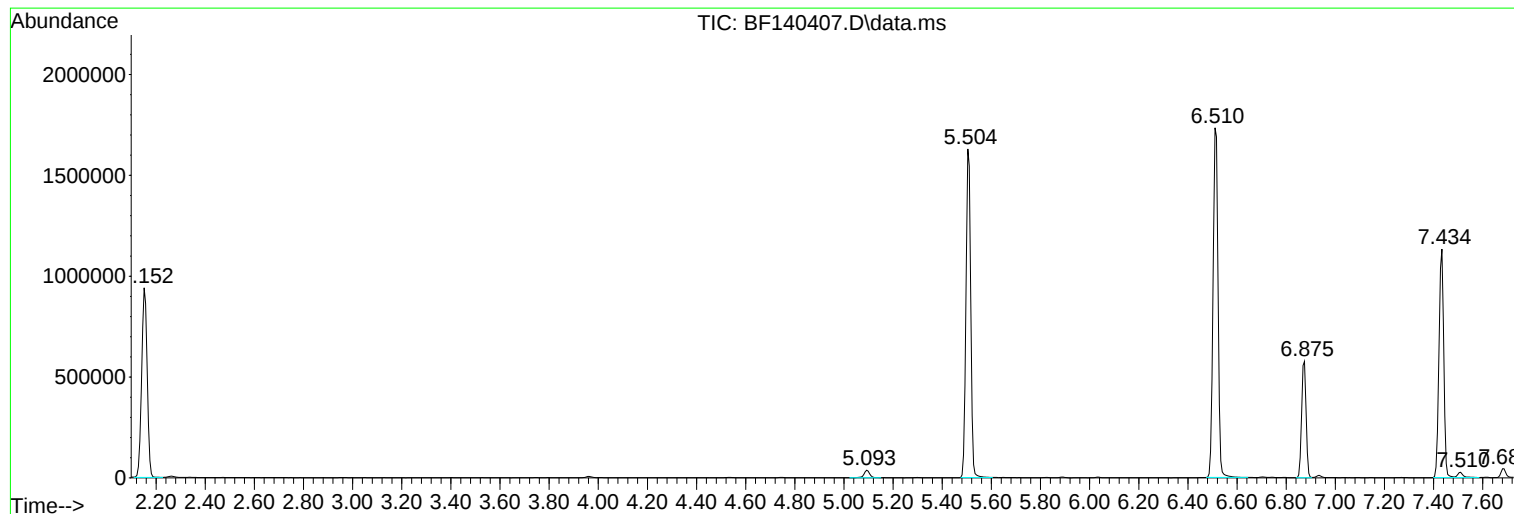
Sum of corrected areas: 20963367

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111524\
Data File : BF140407.D
Acq On : 15 Nov 2024 16:47
Operator : RC/JU
Sample : P4807-13
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-6

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF111324.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\BF111524\
Data File : BF140407.D
Acq On : 15 Nov 2024 16:47
Operator : RC/JU
Sample : P4807-13
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-6

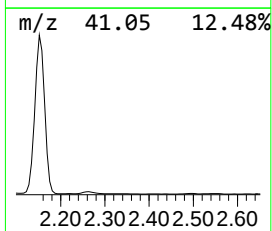
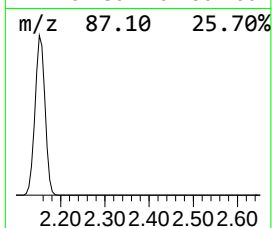
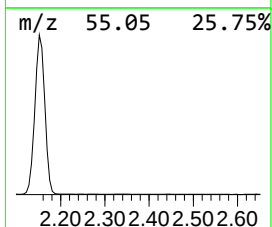
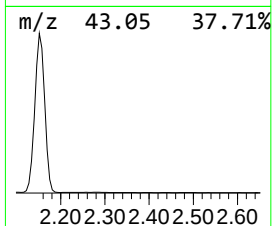
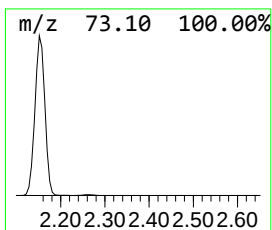
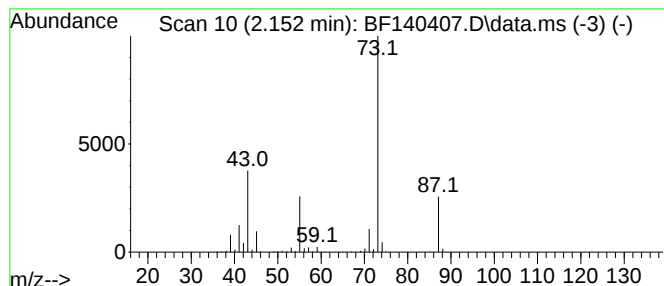
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF111324.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
2.152	40.20 ng	1466990	1,4-Dichlorobenzene-d4	6.875

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	37
4			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17
5			N-Ethylformamide	73	C3H7NO	000627-45-2	9



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111524\
Data File : BF140407.D
Acq On : 15 Nov 2024 16:47
Operator : RC/JU
Sample : P4807-13
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-6

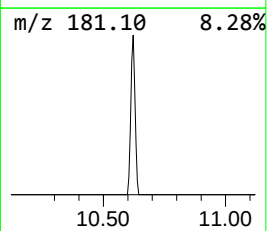
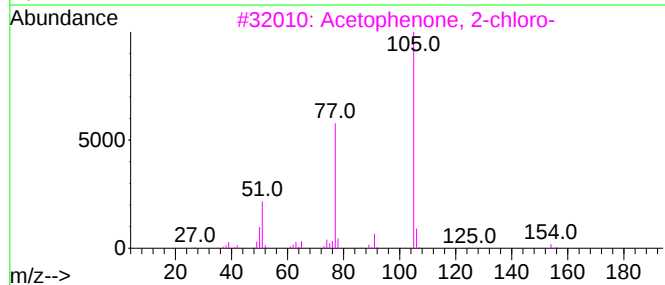
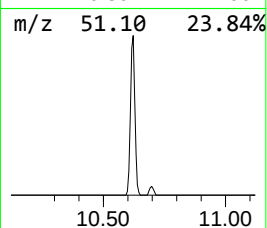
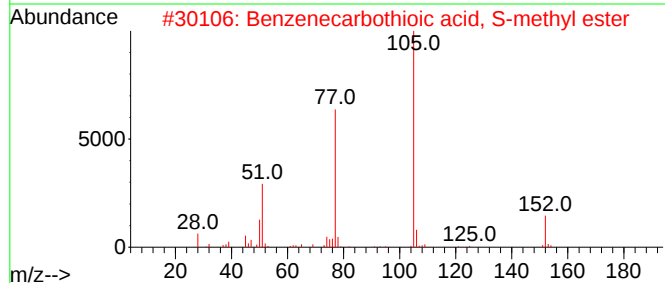
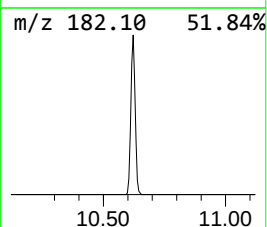
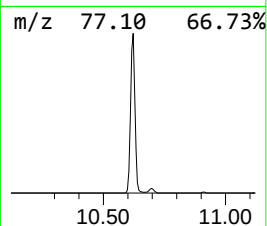
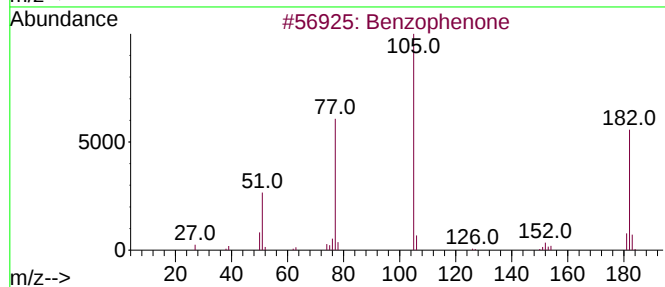
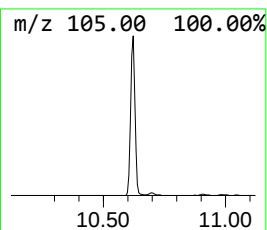
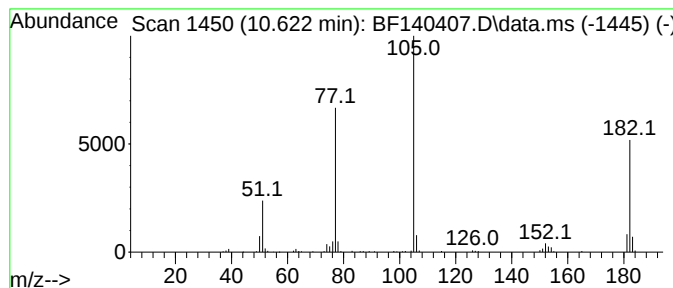
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF111324.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 Benzophenone Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.622	3.84 ng	205276	Acenaphthene-d10	9.910

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	96
2			Benzenecarbothioic acid, S-methy...	152	C8H8OS	005925-68-8	50
3			Acetophenone, 2-chloro-	154	C8H7ClO	000532-27-4	49
4			1-Propanone, 3-chloro-1-phenyl-	168	C9H9ClO	000936-59-4	47
5			Benzenebutanoic acid, .gamma.-oxo-	178	C10H10O3	002051-95-8	47



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111524\
Data File : BF140407.D
Acq On : 15 Nov 2024 16:47
Operator : RC/JU
Sample : P4807-13
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-6

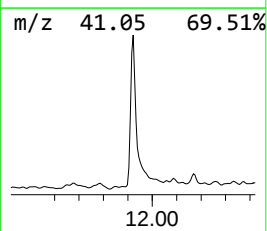
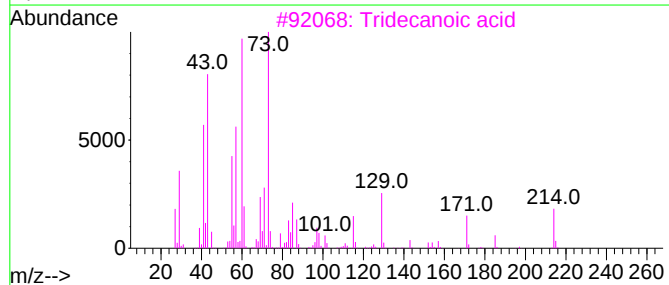
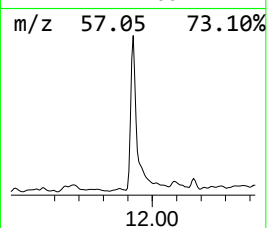
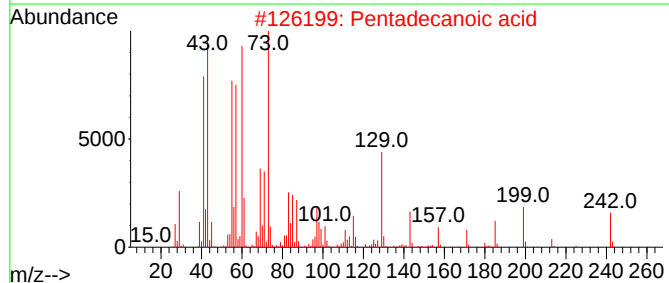
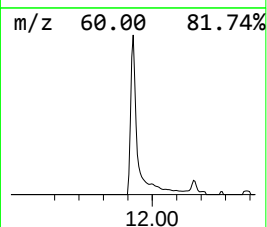
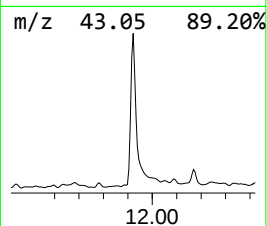
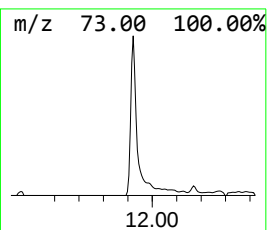
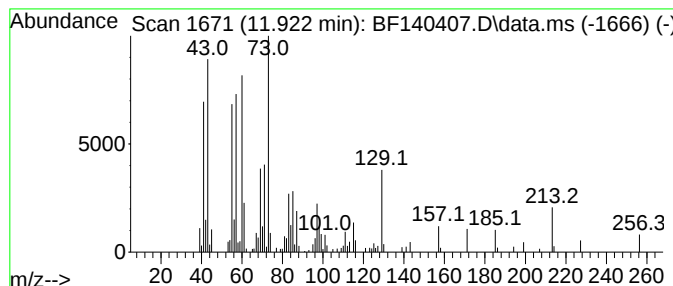
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF111324.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.922	3.88 ng	215983	Phenanthrene-d10	11.398

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	93
3			Tridecanoic acid	214	C13H26O2	000638-53-9	87
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	80
5			Nonanoic acid	158	C9H18O2	000112-05-0	43



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111524\
Data File : BF140407.D
Acq On : 15 Nov 2024 16:47
Operator : RC/JU
Sample : P4807-13
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-6

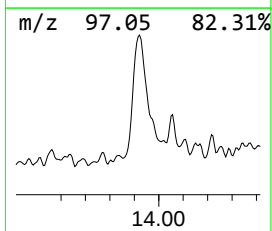
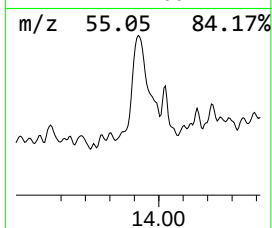
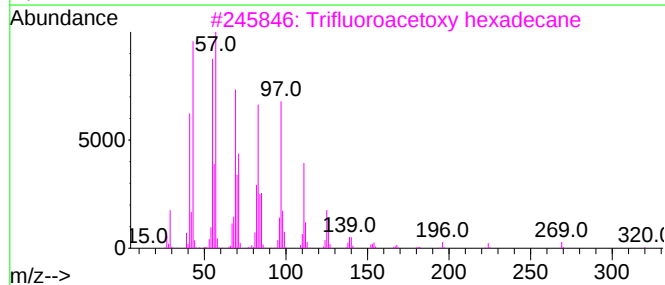
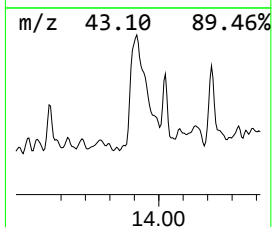
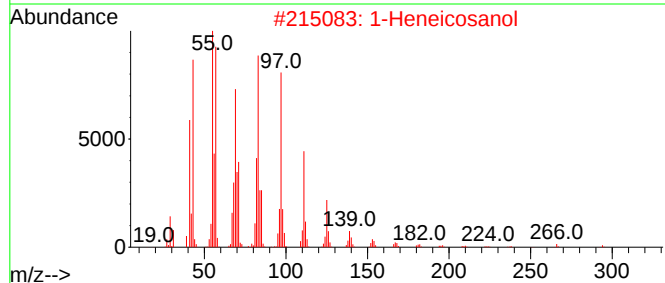
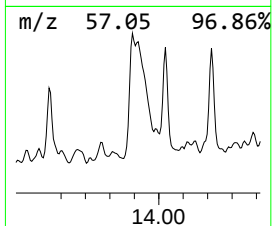
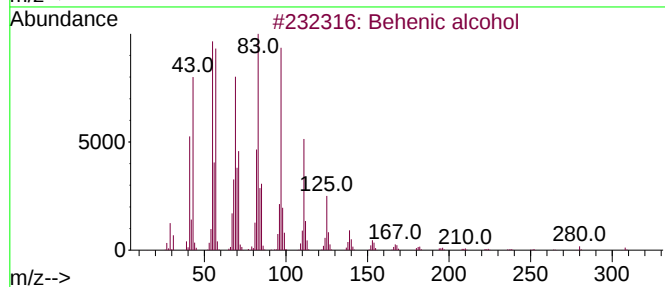
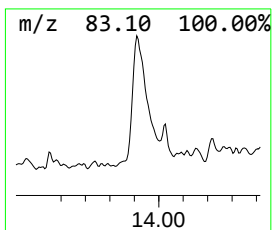
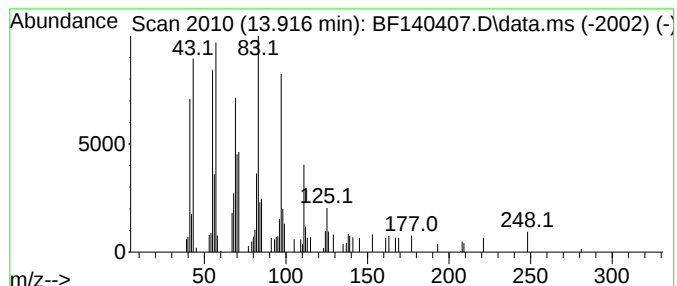
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF111324.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 Behenic alcohol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.916	3.44 ng	127205	Chrysene-d12	14.057

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Behenic alcohol	326	C22H46O	000661-19-8	93
2		1-Heneicosanol	312	C21H44O	015594-90-8	93
3		Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	93
4		n-Nonadecanol-1	284	C19H40O	001454-84-8	90
5		1-Nonadecene	266	C19H38	018435-45-5	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111524\
Data File : BF140407.D
Acq On : 15 Nov 2024 16:47
Operator : RC/JU
Sample : P4807-13
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-6

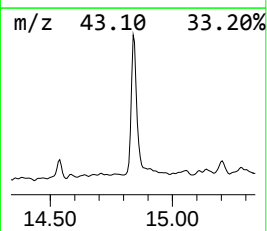
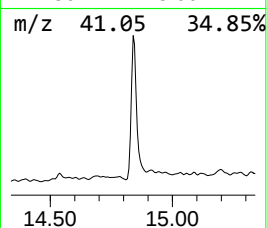
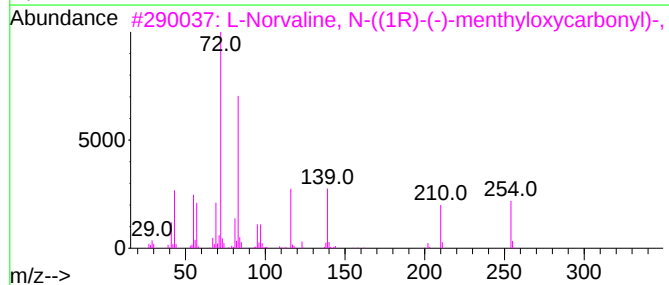
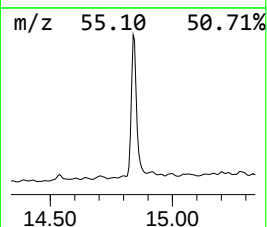
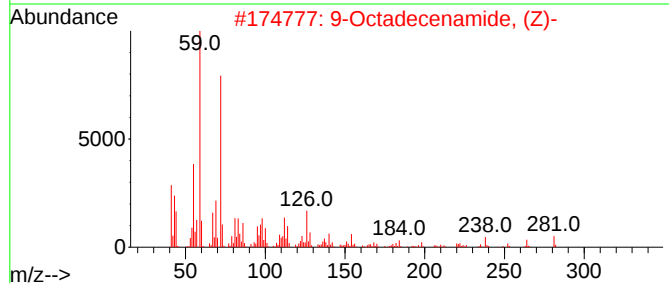
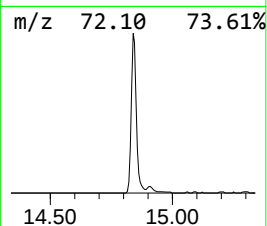
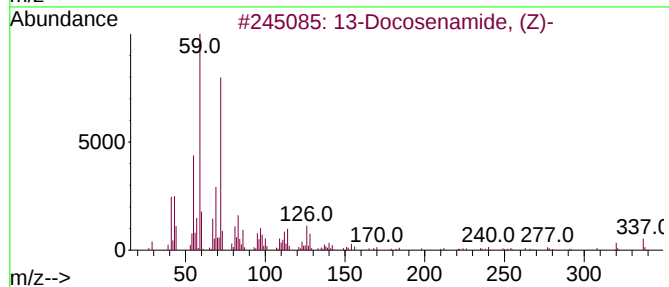
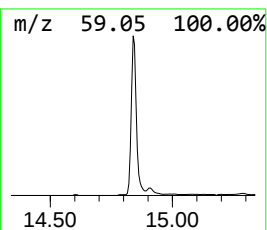
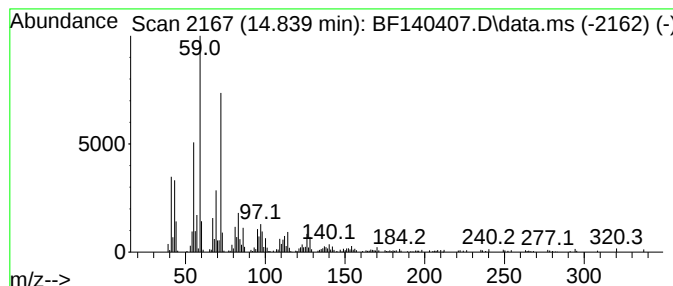
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF111324.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 13-Docosenamide, (Z)- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.839	10.99 ng	404166	Perylene-d12	15.574

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			13-Docosenamide, (Z)-	337	C22H43NO	000112-84-5	98
2			9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	91
3			L-Norvaline, N-((1R)-(-)-menthyl...	383	C22H41NO4	1010392-87-9	35
4			Urea, 1-butyl-3-(propylsulfonyl)...	238	C8H18N2O2S2	024539-91-1	35
5			Acetamide, N-propyl-N-octyl-	213	C13H27NO	1000438-05-6	35



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111524\
Data File : BF140407.D
Acq On : 15 Nov 2024 16:47
Operator : RC/JU
Sample : P4807-13
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-6

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF111324.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	2.152	40.2	ng	1466990	1	6.875	729934	20.0
Benzophenone	10.622	3.8	ng	205276	3	9.910	1068730	20.0
n-Hexadecanoic ...	11.922	3.9	ng	215983	4	11.398	1113970	20.0
Behenic alcohol	13.916	3.4	ng	127205	5	14.057	740181	20.0
13-Docosenamide...	14.839	11.0	ng	404166	6	15.574	735293	20.0