

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110222\
 Data File : BF130937.D
 Acq On : 02 Nov 2022 18:51
 Operator : CG\JU
 Sample : N5395-04
 Misc :
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 S-10-103122

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-BF102722.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF130937.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.252	19	28	37	rVB	555436	714688	32.35%	4.378%
2	2.363	42	47	56	rVB	43507	55304	2.50%	0.339%
3	4.046	328	333	341	rVB	104339	125884	5.70%	0.771%
4	5.157	517	522	530	rVB	404903	498431	22.56%	3.054%
5	5.546	583	588	591	rBV	2151736	2087568	94.49%	12.789%
6	6.545	752	758	761	rBV	2053688	2141870	96.95%	13.122%
7	6.922	818	822	825	rBV	603355	463559	20.98%	2.840%
8	7.316	885	889	898	rVB	62782	65429	2.96%	0.401%
9	7.487	912	918	921	rBV	1433926	1379731	62.45%	8.453%
10	8.104	1020	1023	1036	rBV	109890	233128	10.55%	1.428%
11	8.204	1036	1040	1043	rBV	622305	589581	26.69%	3.612%
12	9.286	1219	1224	1227	rBV	2676037	2209267	100.00%	13.535%
13	9.969	1336	1340	1343	rVB	798923	639007	28.92%	3.915%
14	10.757	1470	1474	1477	rBV	1491395	1272278	57.59%	7.795%
15	10.804	1479	1482	1488	rVB	51942	47366	2.14%	0.290%
16	11.457	1590	1593	1596	rBV	641344	575895	26.07%	3.528%
17	11.480	1596	1597	1600	rVV	77891	52070	2.36%	0.319%
18	11.522	1601	1604	1609	rVB2	28689	32416	1.47%	0.199%
19	11.845	1656	1659	1662	rBV	35861	29343	1.33%	0.180%
20	12.674	1797	1800	1803	rVB	136593	105324	4.77%	0.645%
21	12.904	1834	1839	1843	rBV	103741	113189	5.12%	0.693%
22	13.051	1857	1864	1867	rBV	1685694	1434644	64.94%	8.789%
23	13.945	2014	2016	2020	rVB3	25711	26059	1.18%	0.160%
24	14.027	2025	2030	2031	rBV5	19076	32240	1.46%	0.198%
25	14.104	2037	2043	2046	rBV2	397584	423688	19.18%	2.596%
26	14.133	2046	2048	2053	rVB	53477	45584	2.06%	0.279%
27	15.168	2221	2224	2227	rBV	43937	61902	2.80%	0.379%
28	15.245	2233	2237	2241	rBV	35160	46708	2.11%	0.286%
29	15.486	2275	2278	2284	rVB	32129	45281	2.05%	0.277%
30	15.551	2285	2289	2295	rVB	39553	54229	2.45%	0.332%
31	15.621	2296	2301	2305	rBV	303440	405646	18.36%	2.485%
32	15.863	2337	2342	2348	rVB2	97317	137252	6.21%	0.841%
33	16.104	2380	2383	2388	rVB2	27458	37770	1.71%	0.231%
34	16.957	2522	2528	2537	rVB3	48381	112415	5.09%	0.689%
35	17.145	2557	2560	2565	rVB2	16871	27988	1.27%	0.171%

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110222\
Data File : BF130937.D
Acq On : 02 Nov 2022 18:51
Operator : CG\JU
Sample : N5395-04
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
S-10-103122

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-BF102722.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

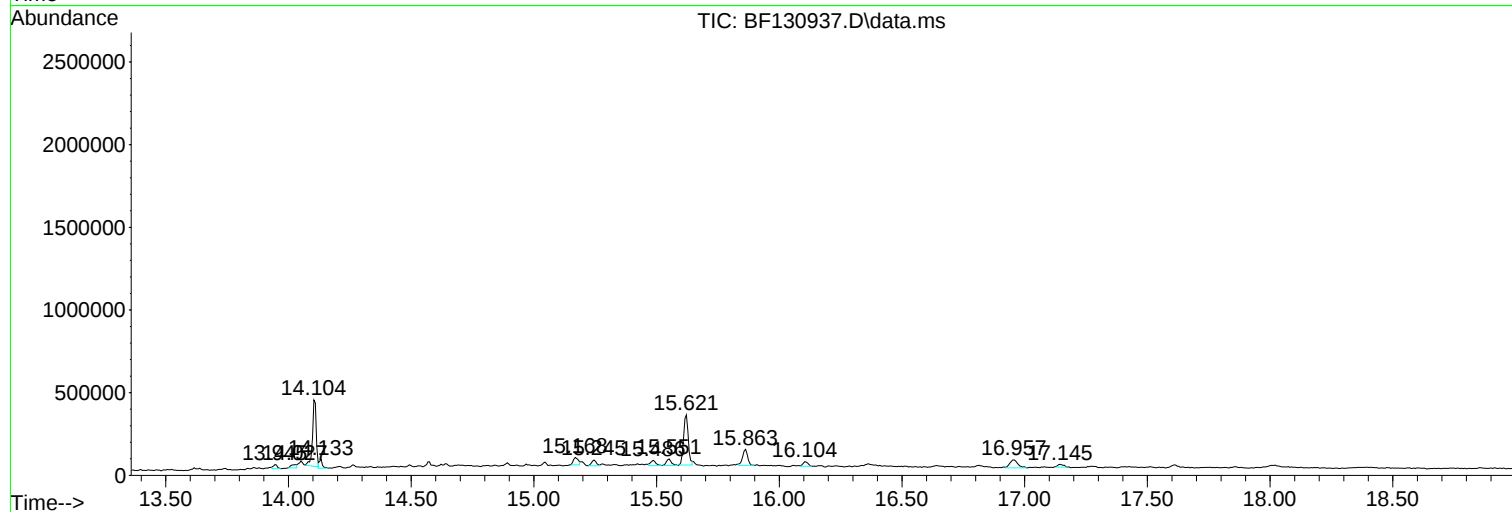
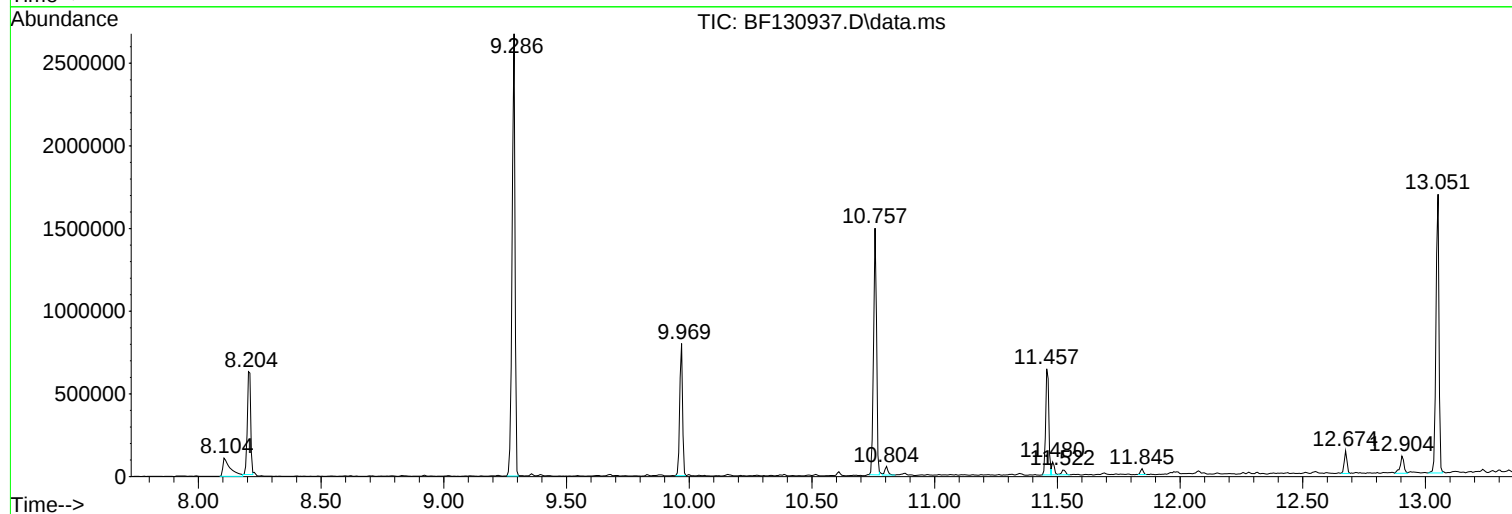
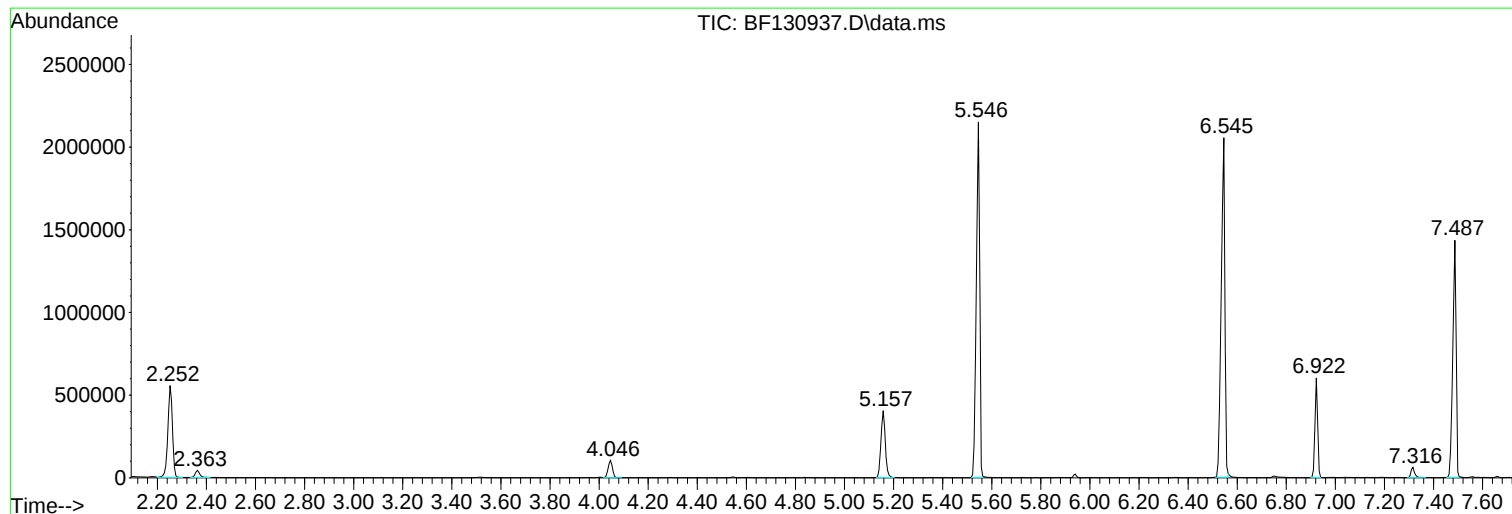
Sum of corrected areas: 16322734

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110222\
Data File : BF130937.D
Acq On : 02 Nov 2022 18:51
Operator : CG\JU
Sample : N5395-04
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
S-10-103122

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF102722.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\BF110222\
Data File : BF130937.D
Acq On : 02 Nov 2022 18:51
Operator : CG\JU
Sample : N5395-04
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
S-10-103122

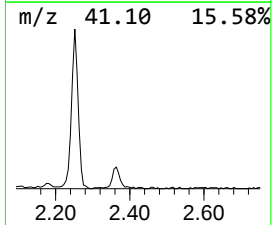
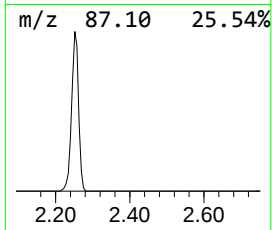
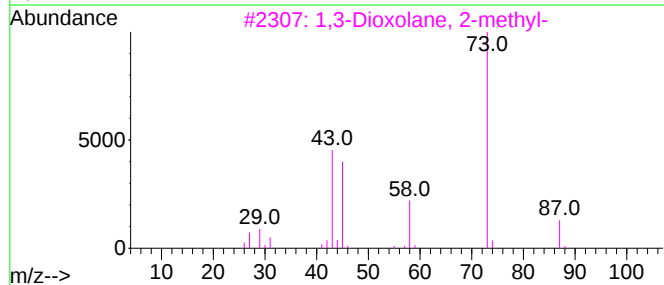
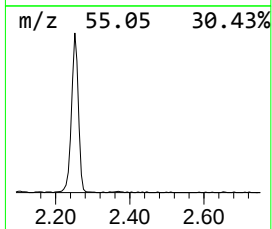
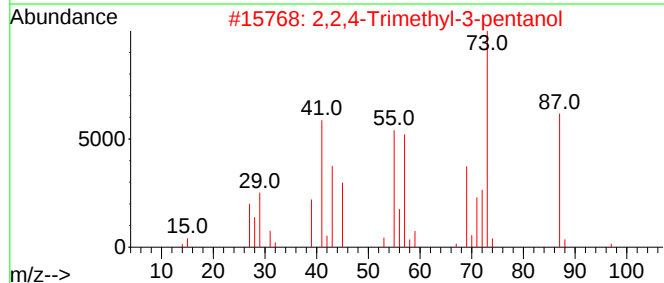
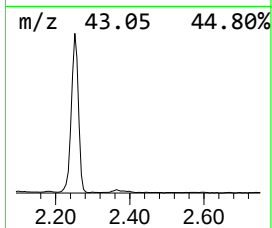
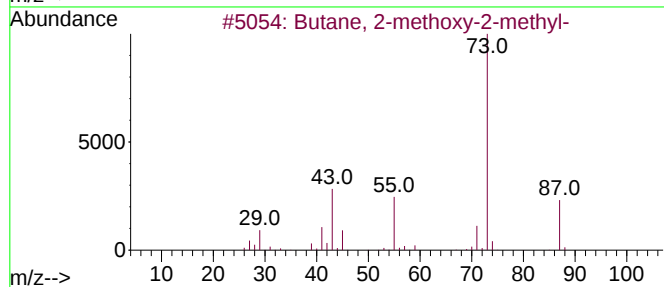
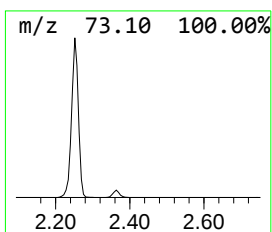
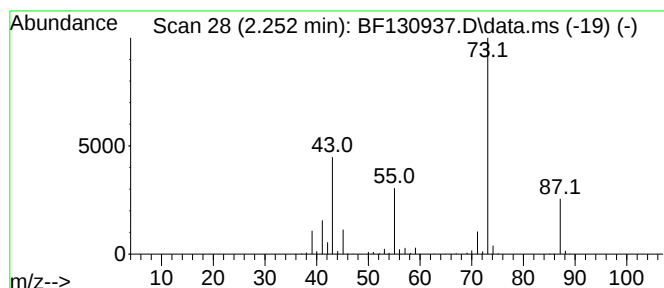
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF102722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
2.252	30.83 ng	714688	1,4-Dichlorobenzene-d4	6.922

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	37
4		Boronic acid, ethyl-, dimethyl e...	102	C4H11BO2	007318-82-3	17
5		3-Pentanol, 3-methyl-	102	C6H14O	000077-74-7	17



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110222\
Data File : BF130937.D
Acq On : 02 Nov 2022 18:51
Operator : CG\JU
Sample : N5395-04
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
S-10-103122

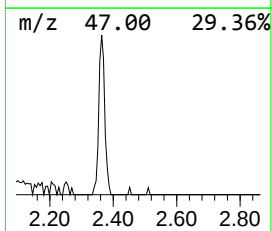
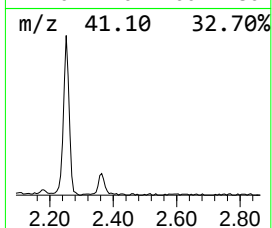
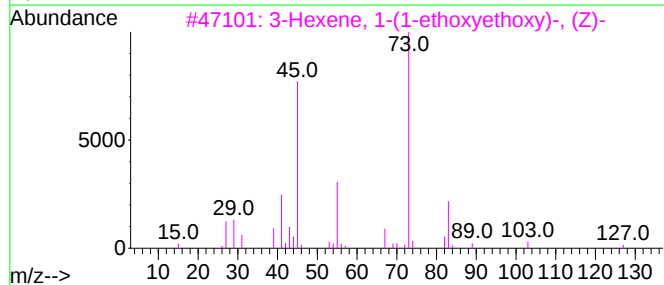
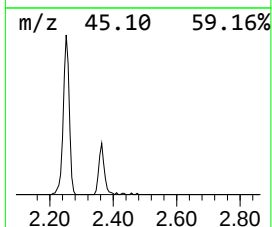
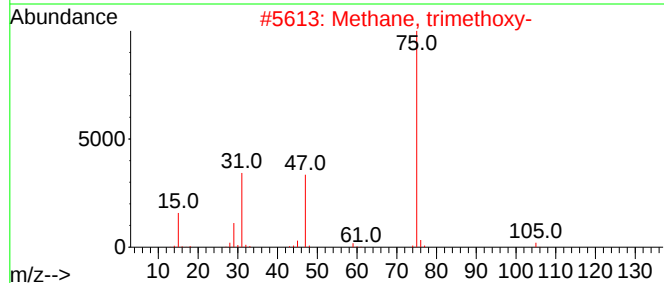
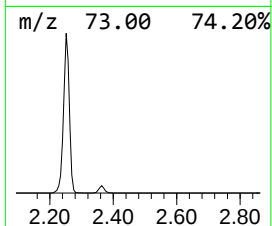
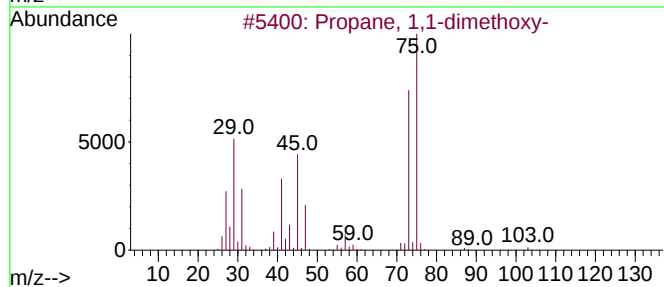
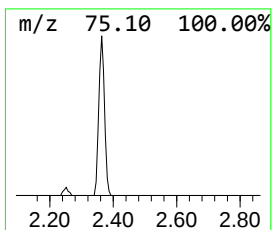
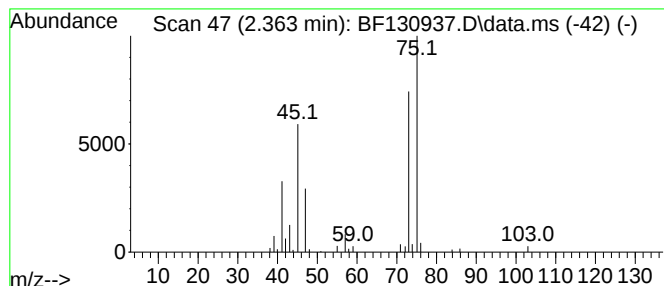
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF102722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 Propane, 1,1-dimethoxy- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.363	2.39 ng	55304	1,4-Dichlorobenzene-d4	6.922

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propane, 1,1-dimethoxy-	104	C5H12O2	004744-10-9	83
2			Methane, trimethoxy-	106	C4H10O3	000149-73-5	28
3			3-Hexene, 1-(1-ethoxyethoxy)-, (Z)-	172	C10H20O2	028069-74-1	10
4			Methane, isothiocyanato-	73	C2H3NS	000556-61-6	9
5			2-Propanol, 1-methoxy-	90	C4H10O2	000107-98-2	9



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110222\
Data File : BF130937.D
Acq On : 02 Nov 2022 18:51
Operator : CG\JU
Sample : N5395-04
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
S-10-103122

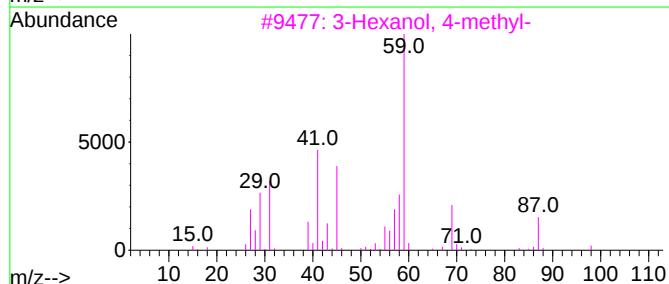
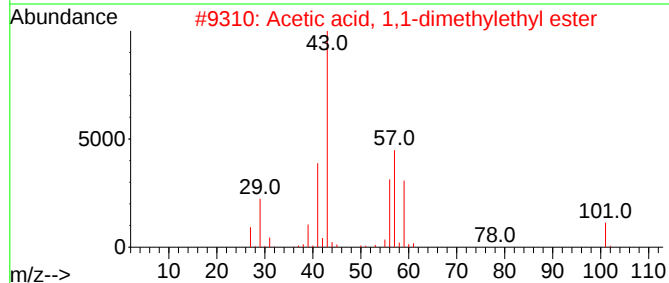
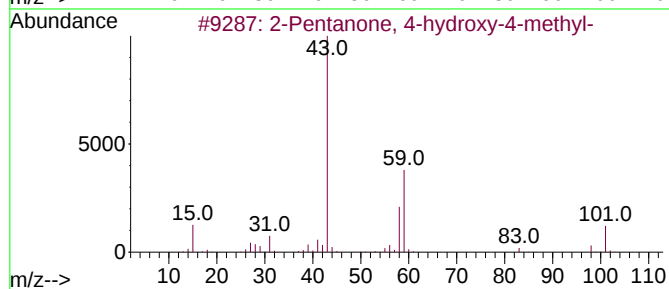
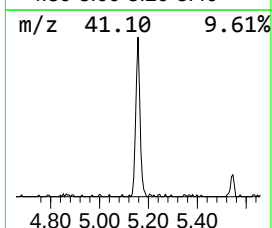
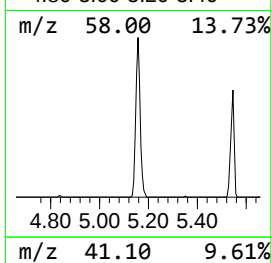
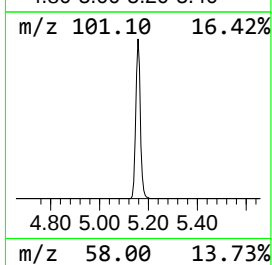
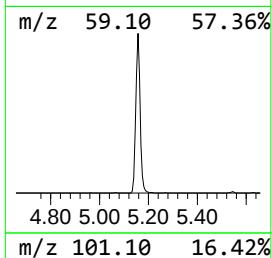
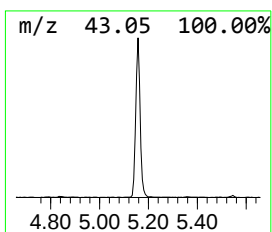
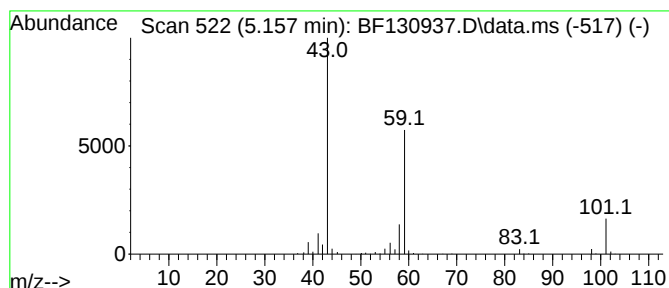
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF102722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.157	21.50 ng	498431	1,4-Dichlorobenzene-d4	6.922

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50		
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	38		
3	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33		
4	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28		
5	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25		



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110222\
Data File : BF130937.D
Acq On : 02 Nov 2022 18:51
Operator : CG\JU
Sample : N5395-04
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
S-10-103122

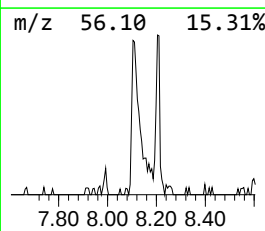
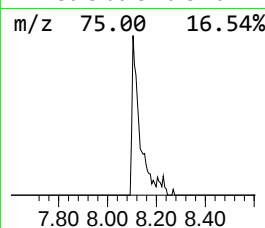
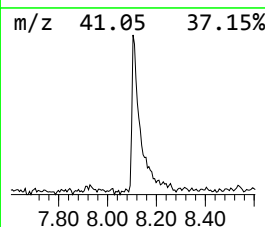
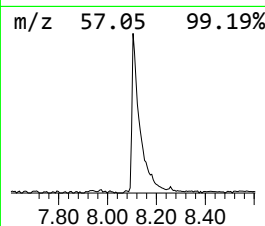
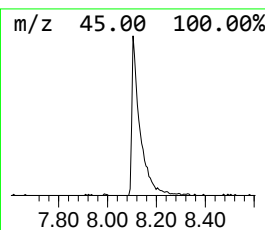
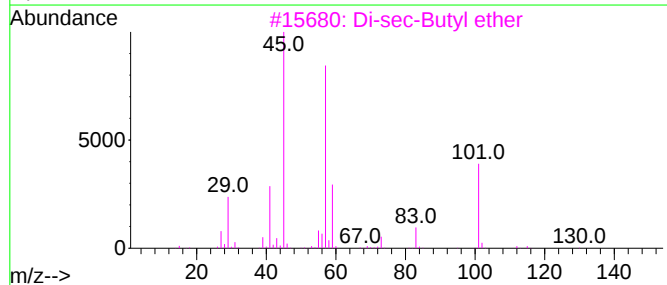
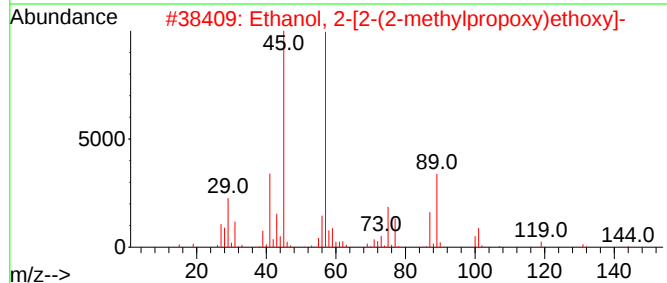
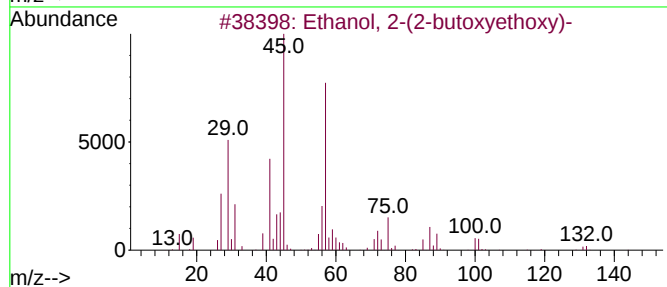
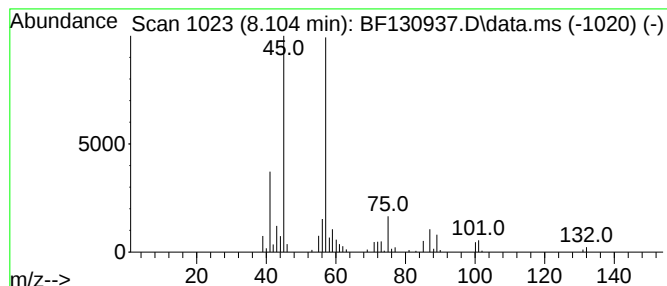
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF102722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.104	7.91 ng	233128	Naphthalene-d8	8.210

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	78
2			Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	56
3			Di-sec-Butyl ether	130	C8H18O	006863-58-7	53
4			Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	50
5			Ethanol, 2-[2-(2-butoxyethoxy)et...	206	C10H22O4	000143-22-6	50



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110222\
Data File : BF130937.D
Acq On : 02 Nov 2022 18:51
Operator : CG\JU
Sample : N5395-04
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
S-10-103122

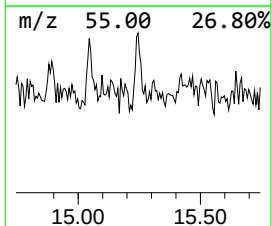
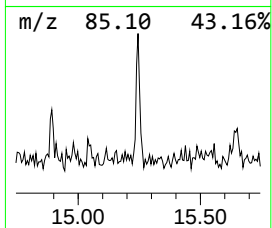
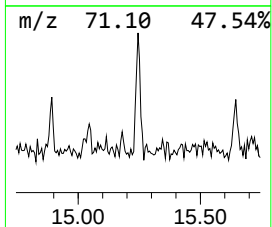
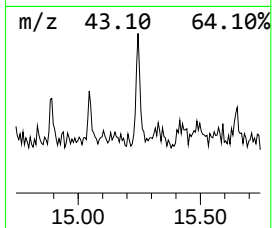
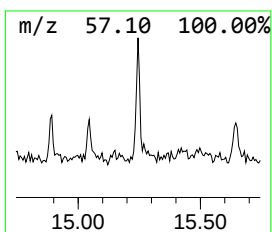
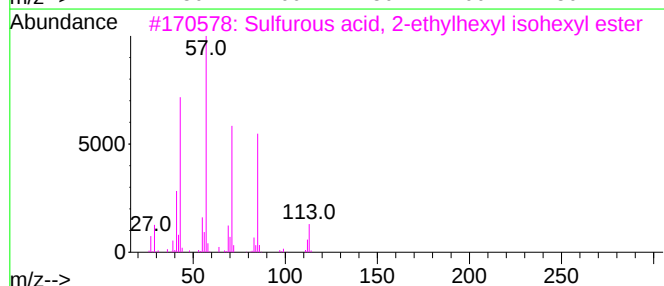
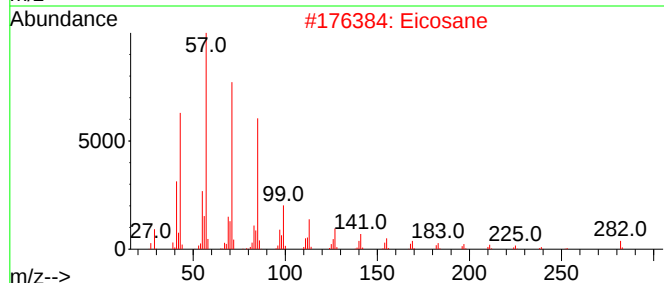
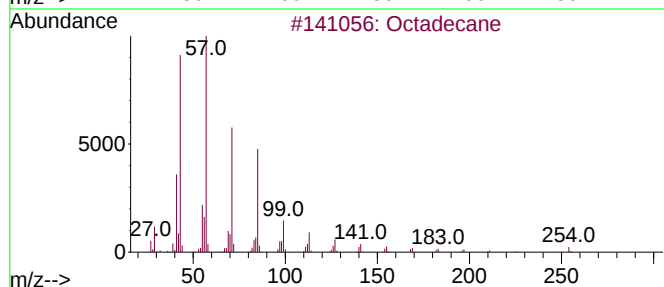
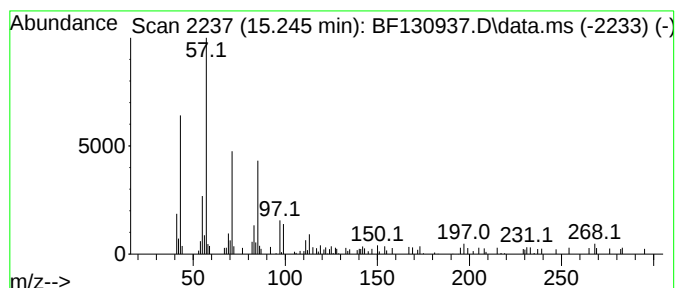
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF102722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Octadecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.245	2.30 ng	46708	Perylene-d12	15.621

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecane	254	C18H38	000593-45-3	80
2			Eicosane	282	C20H42	000112-95-8	72
3			Sulfurous acid, 2-ethylhexyl iso...	278	C14H30O3S	1000309-19-0	59
4			Nonadecane	268	C19H40	000629-92-5	52
5			Sulfurous acid, 2-propyl tridecy...	306	C16H34O3S	1000309-12-4	49



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110222\
Data File : BF130937.D
Acq On : 02 Nov 2022 18:51
Operator : CG\JU
Sample : N5395-04
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
S-10-103122

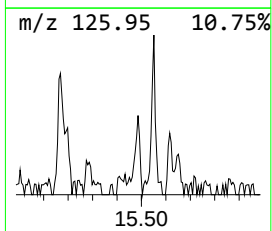
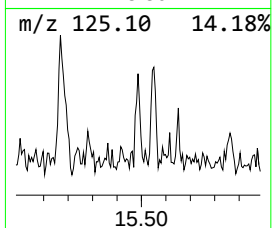
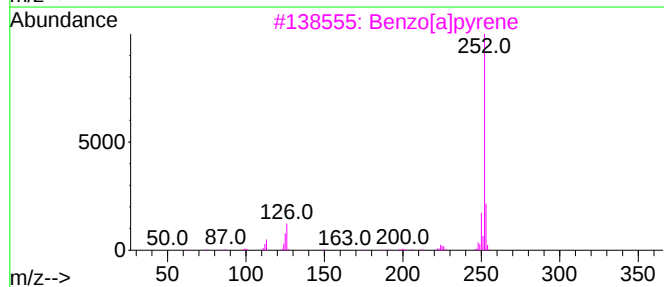
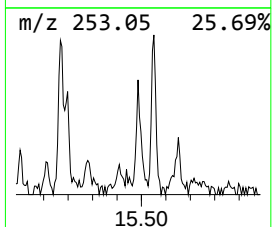
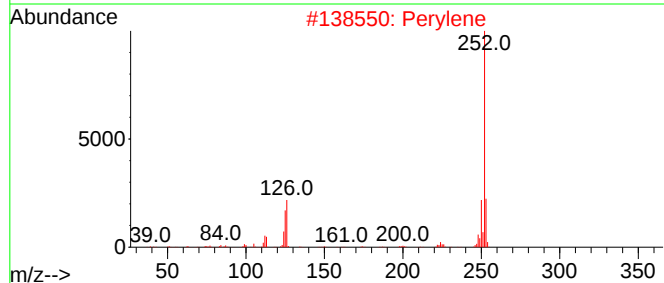
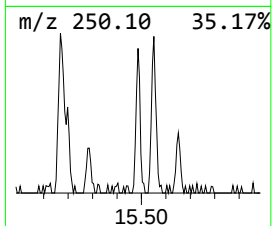
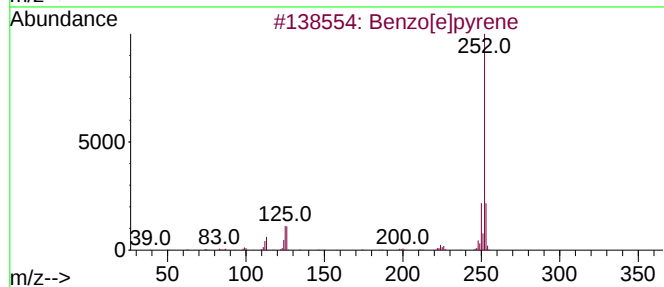
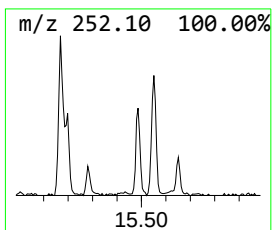
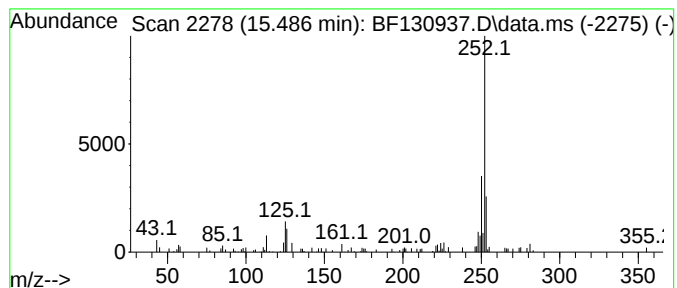
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF102722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Benzo[e]pyrene Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.486	2.23 ng	45281	Perylene-d12	15.621

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzo[e]pyrene	252	C20H12	000192-97-2	76
2			Perylene	252	C20H12	000198-55-0	70
3			Benzo[a]pyrene	252	C20H12	000050-32-8	68
4			Benzo[b]fluoranthene	252	C20H12	000205-99-2	62
5			Benzo[k]fluoranthene	252	C20H12	000207-08-9	62



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110222\
Data File : BF130937.D
Acq On : 02 Nov 2022 18:51
Operator : CG\JU
Sample : N5395-04
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
S-10-103122

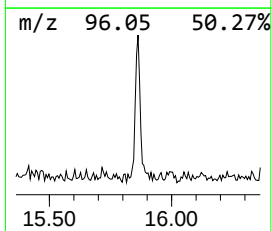
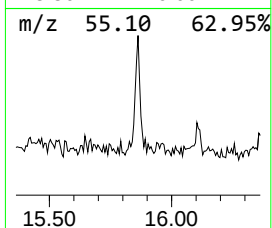
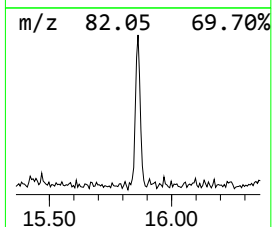
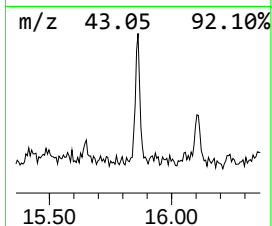
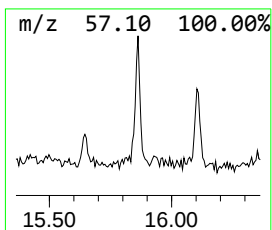
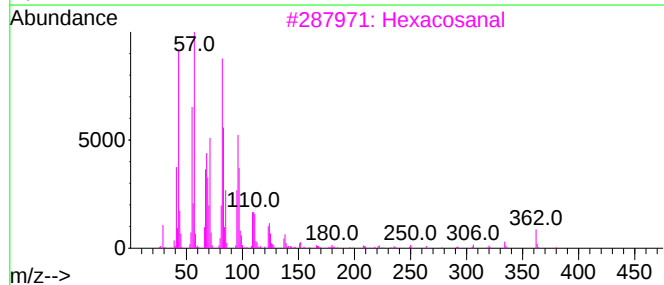
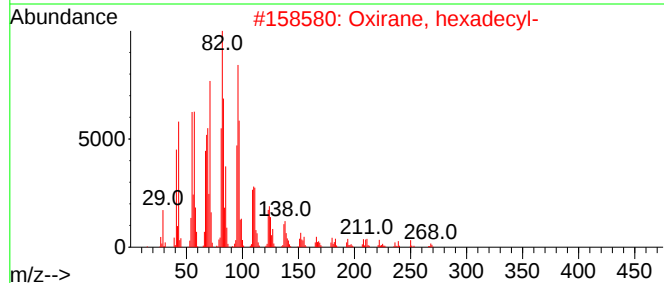
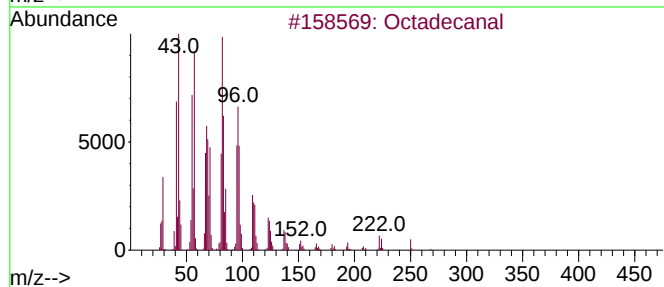
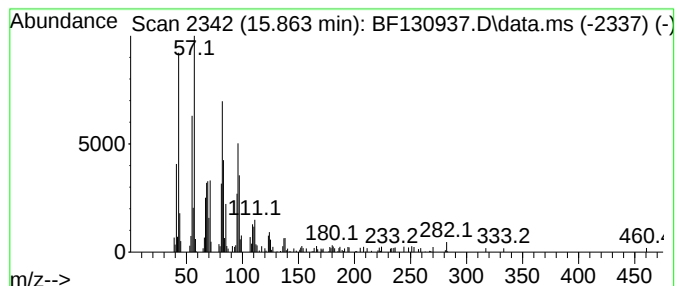
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF102722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Octadecanal Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.863	6.77 ng	137252	Perylene-d12	15.621

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanal	268	C18H36O	000638-66-4	93
2			Oxirane, hexadecyl-	268	C18H36O	007390-81-0	91
3			Hexacosanal	380	C26H52O	026627-85-0	90
4			1,16-Hexadecanediol	258	C16H34O2	007735-42-4	87
5			1,19-Eicosadiene	278	C20H38	014811-95-1	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110222\
Data File : BF130937.D
Acq On : 02 Nov 2022 18:51
Operator : CG\JU
Sample : N5395-04
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
S-10-103122

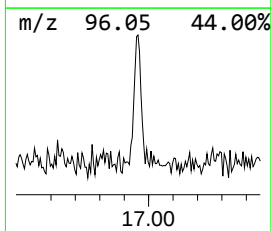
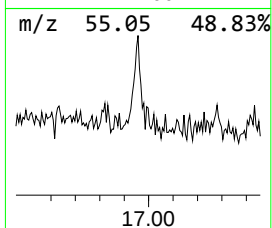
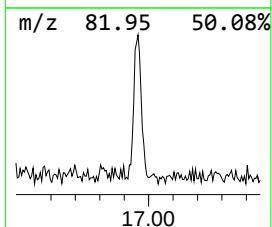
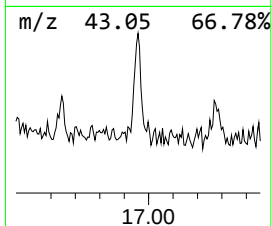
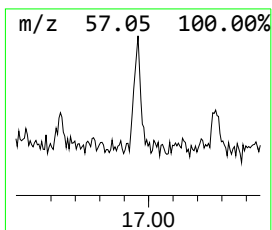
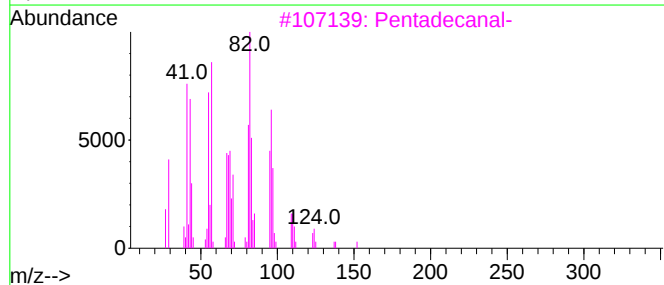
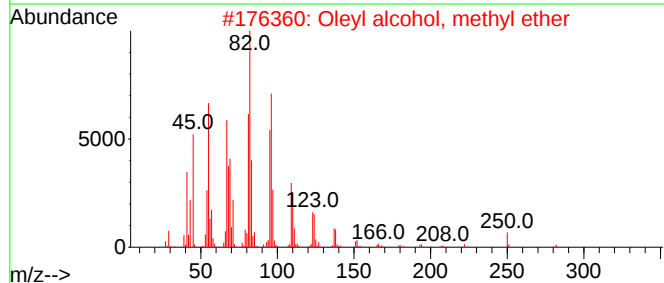
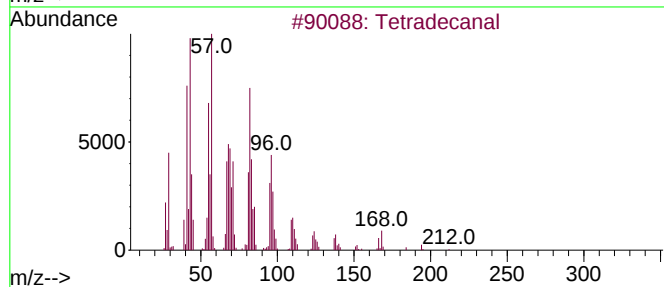
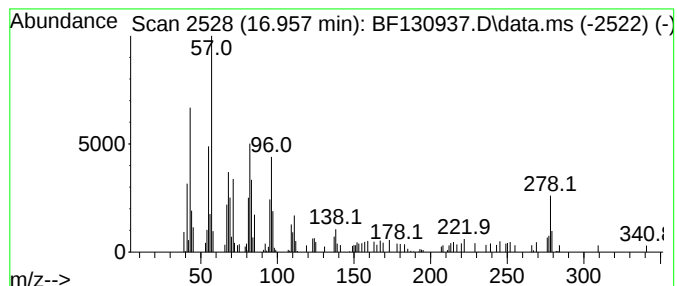
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF102722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Tetradecanal Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.957	5.54 ng	112415	Perylene-d12	15.621

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Tetradecanal	212	C14H28O	000124-25-4	64
2		Oleyl alcohol, methyl ether	282	C19H38O	1010352-68-0	55
3		Pentadecanal-	226	C15H30O	002765-11-9	52
4		Octadecanal	268	C18H36O	000638-66-4	49
5		Tetracosanal	352	C24H48O	057866-08-7	46



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110222\
Data File : BF130937.D
Acq On : 02 Nov 2022 18:51
Operator : CG\JU
Sample : N5395-04
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
S-10-103122

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF102722.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...	2.252	30.8	ng	714688	1	6.922	463559	20.0
Propane, 1,1-di...	2.363	2.4	ng	55304	1	6.922	463559	20.0
2-Pentanone, 4-...	5.157	21.5	ng	498431	1	6.922	463559	20.0
Ethanol, 2-(2-b...	8.104	7.9	ng	233128	2	8.210	589581	20.0
Octadecane	15.245	2.3	ng	46708	6	15.621	405646	20.0
Benzo[e]pyrene	15.486	2.2	ng	45281	6	15.621	405646	20.0
Octadecanal	15.863	6.8	ng	137252	6	15.621	405646	20.0
Tetradecanal	16.957	5.5	ng	112415	6	15.621	405646	20.0