

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF103122\
 Data File : BF130877.D
 Acq On : 31 Oct 2022 13:54
 Operator : CG\JU
 Sample : N5234-02
 Misc :
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 LSP-SS-03-03-05

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: BF130877.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.258	23	29	37	rVB	930632	1257652	61.42%	7.655%
2	5.169	519	524	533	rVB	312500	359019	17.53%	2.185%
3	5.557	585	590	593	rBV	1861854	1679610	82.02%	10.223%
4	6.557	755	760	763	rBV	1828917	1830990	89.42%	11.145%
5	6.940	821	825	828	rBV	663419	514281	25.11%	3.130%
6	7.504	911	921	924	rBV	1149639	1175944	57.43%	7.158%
7	8.140	1024	1029	1039	rBV2	28820	68587	3.35%	0.417%
8	8.228	1039	1044	1047	rBV	712887	657290	32.10%	4.001%
9	9.304	1221	1227	1230	rBV	2433712	2047739	100.00%	12.464%
10	9.986	1338	1343	1346	rBV	907570	744004	36.33%	4.528%
11	10.192	1371	1378	1381	rVB3	13869	23493	1.15%	0.143%
12	10.533	1431	1436	1440	rBV	24432	23981	1.17%	0.146%
13	10.775	1473	1477	1481	rBV	1247366	1098172	53.63%	6.684%
14	11.480	1593	1597	1599	rBV	924714	736307	35.96%	4.482%
15	11.504	1599	1601	1604	rVV	128724	99362	4.85%	0.605%
16	11.551	1604	1609	1612	rVB2	50924	64123	3.13%	0.390%
17	11.992	1678	1684	1690	rBV3	67351	111198	5.43%	0.677%
18	12.098	1698	1702	1704	rBV	31346	35196	1.72%	0.214%
19	12.698	1800	1804	1809	rVB	183748	165902	8.10%	1.010%
20	12.927	1837	1843	1846	rBV	173536	178260	8.71%	1.085%
21	13.069	1863	1867	1870	rVB	1839798	1511955	73.84%	9.203%
22	13.357	1912	1916	1919	rBV2	19527	24970	1.22%	0.152%
23	13.545	1944	1948	1953	rVB3	28512	35617	1.74%	0.217%
24	13.639	1959	1964	1966	rBV2	20103	25500	1.25%	0.155%
25	13.739	1972	1981	1982	rBV7	30412	73436	3.59%	0.447%
26	13.969	2015	2020	2027	rBV5	49268	106201	5.19%	0.646%
27	14.127	2041	2047	2050	rBV	528282	527110	25.74%	3.208%
28	14.151	2050	2051	2056	rVB	64787	52946	2.59%	0.322%
29	14.221	2058	2063	2068	rBV	132533	137362	6.71%	0.836%
30	14.592	2115	2126	2133	rBV	79408	250685	12.24%	1.526%
31	14.898	2174	2178	2192	rBV2	95507	165227	8.07%	1.006%
32	14.992	2192	2194	2199	rVB	37737	39228	1.92%	0.239%
33	15.192	2225	2228	2232	rBV2	46550	67529	3.30%	0.411%
34	15.510	2279	2282	2288	rBV	28301	37428	1.83%	0.228%
35	15.574	2290	2293	2300	rVB	42787	55226	2.70%	0.336%
36	15.645	2300	2305	2309	rBV2	322376	447992	21.88%	2.727%

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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

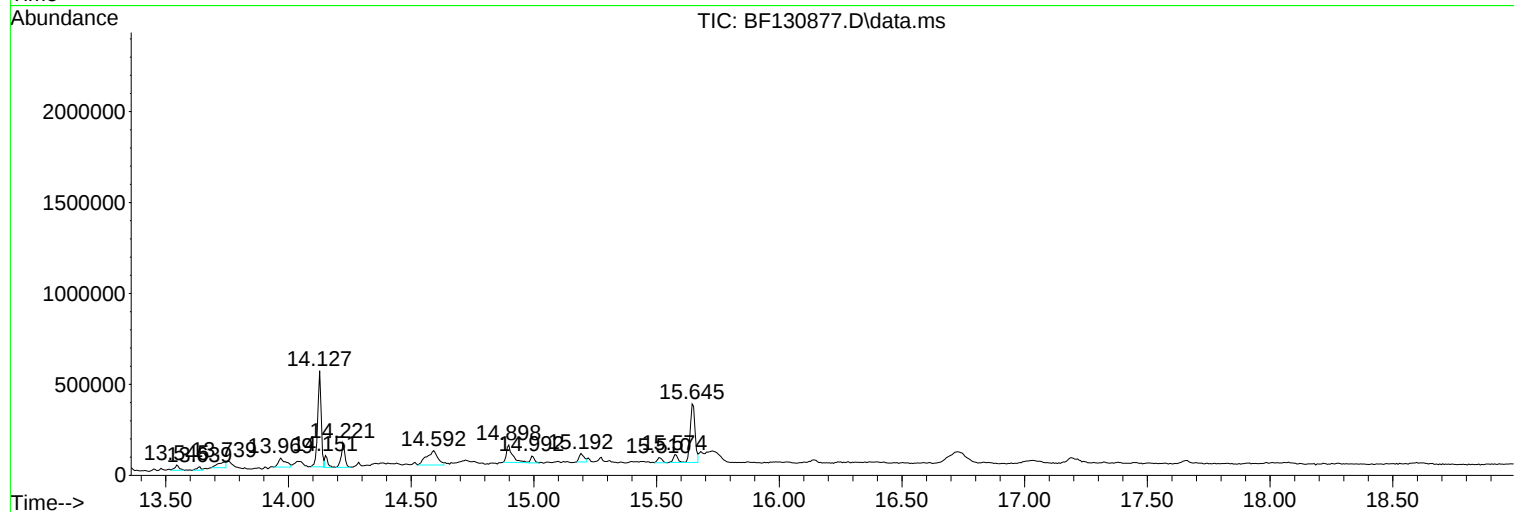
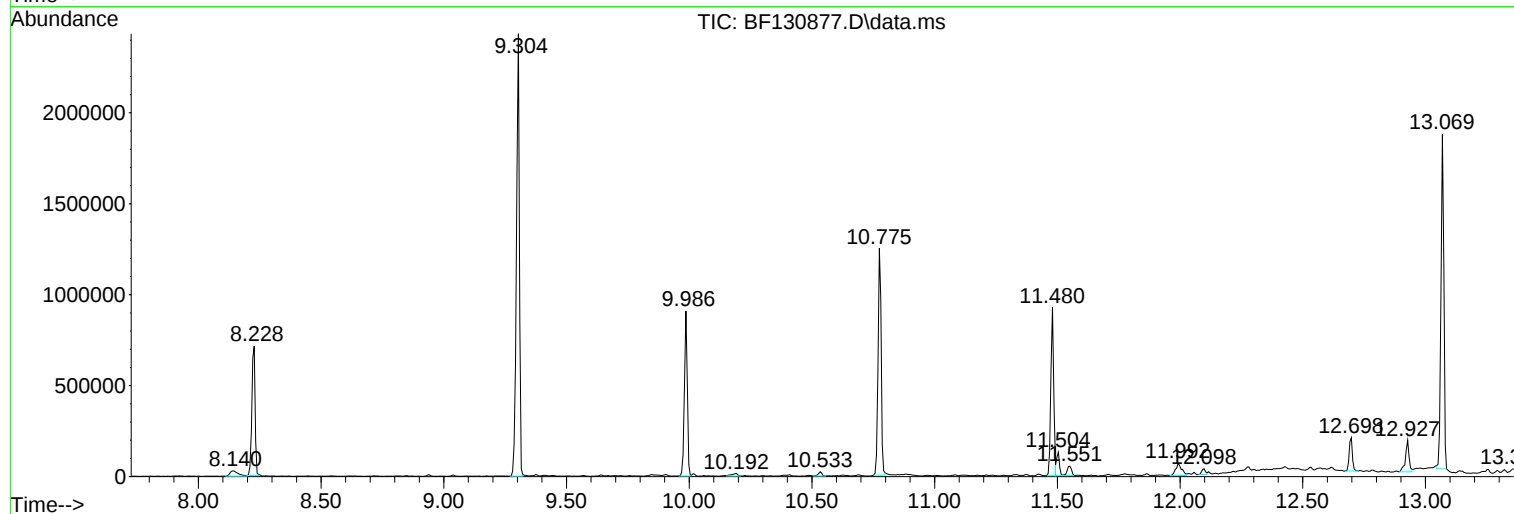
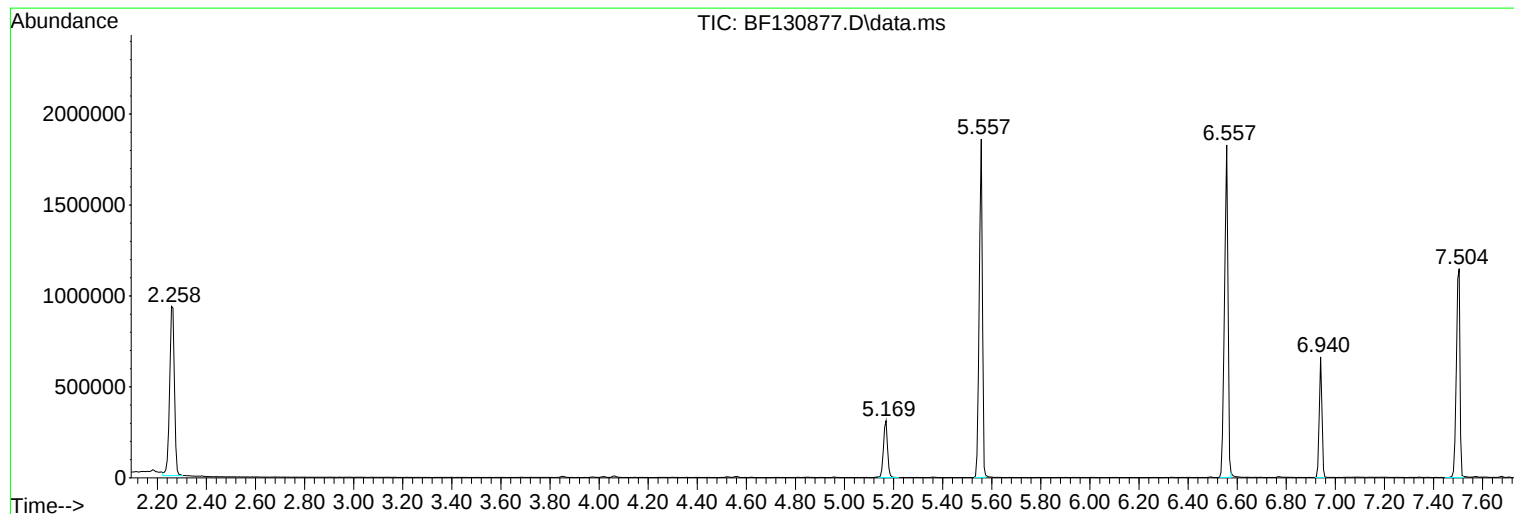
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF102722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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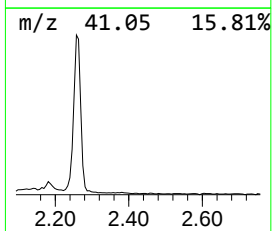
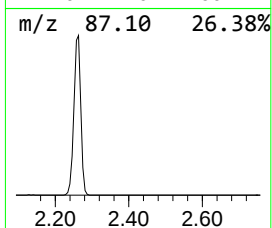
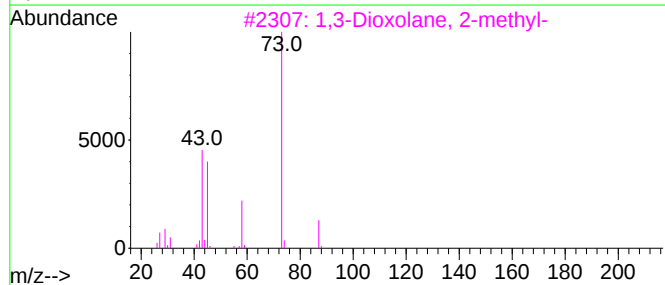
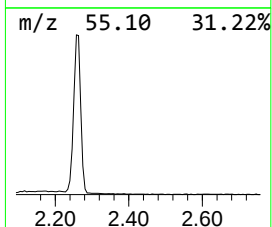
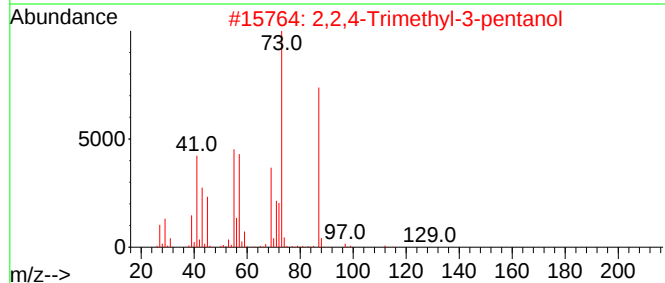
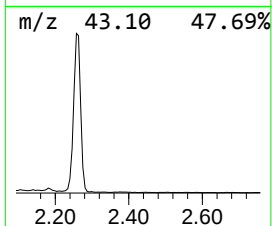
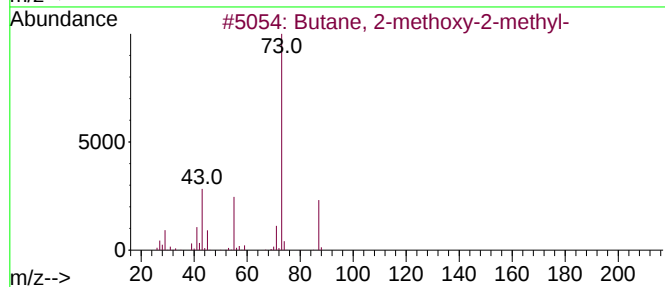
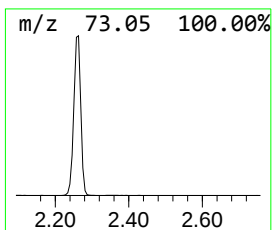
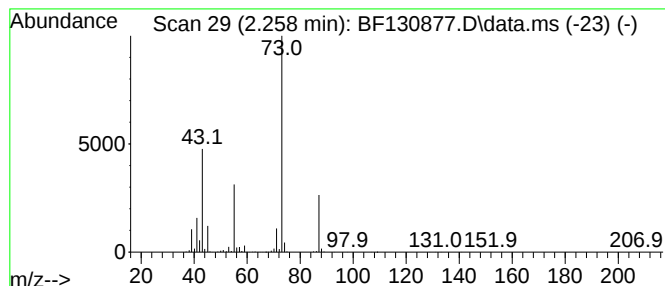
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF102722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
2.258	48.91 ng	1257650	1,4-Dichlorobenzene-d4	6.940

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			Silane, tetramethyl-	88	C4H12Si	000075-76-3	17
5			Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	9



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Instrument :
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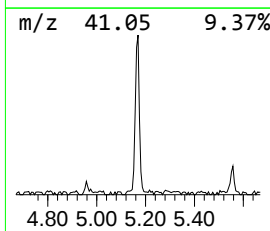
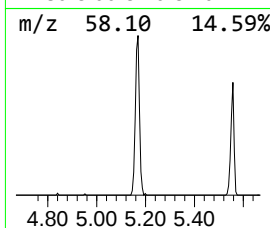
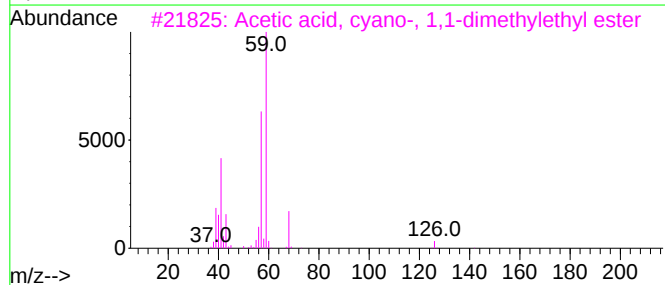
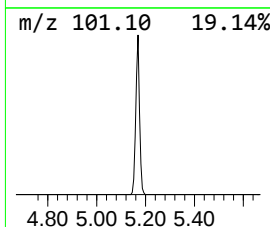
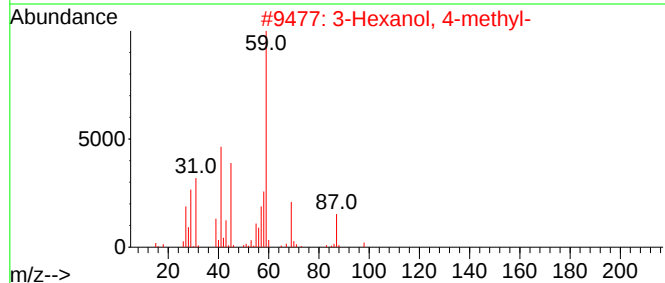
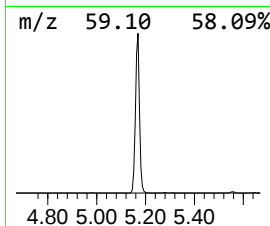
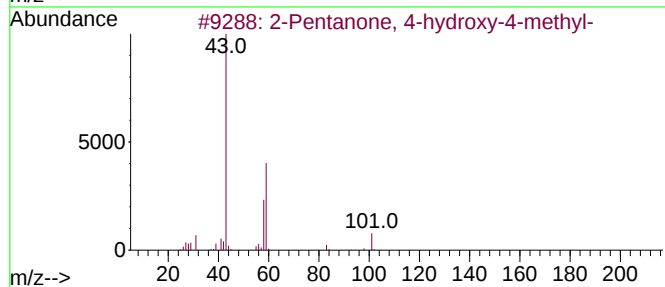
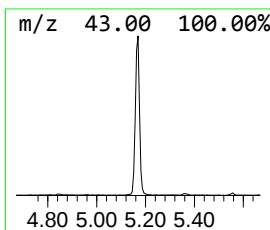
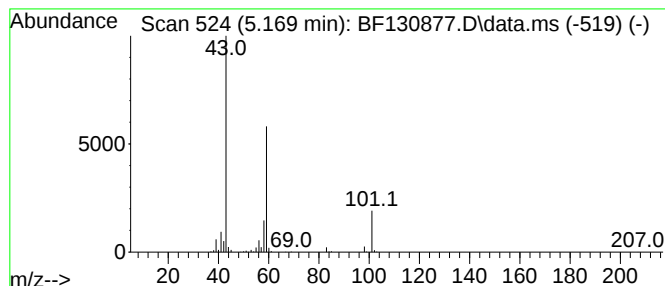
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TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.169	13.96 ng	359019	1,4-Dichlorobenzene-d4	6.940

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2		3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	28
3		Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
4		1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
5		2-Propanone, 1-(1-methylethoxy)-	116	C6H12O2	042781-12-4	9



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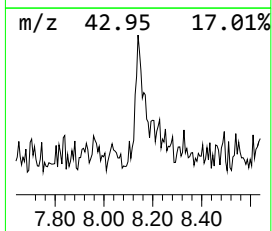
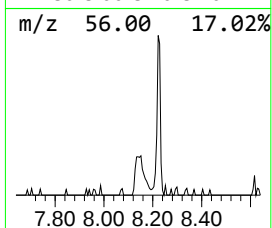
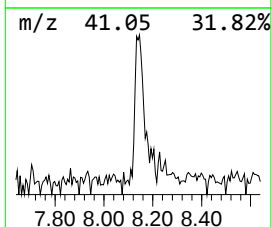
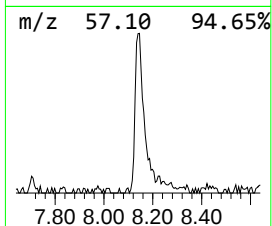
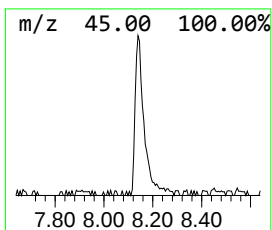
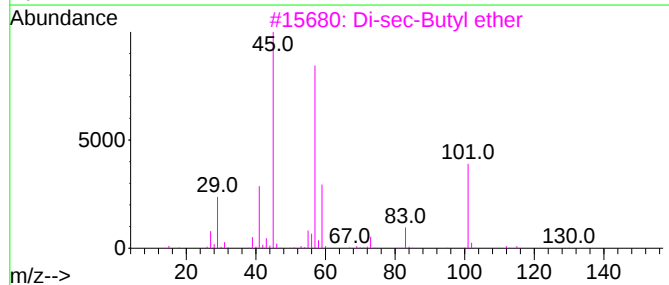
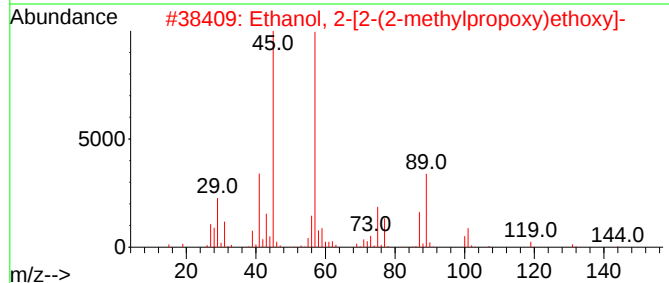
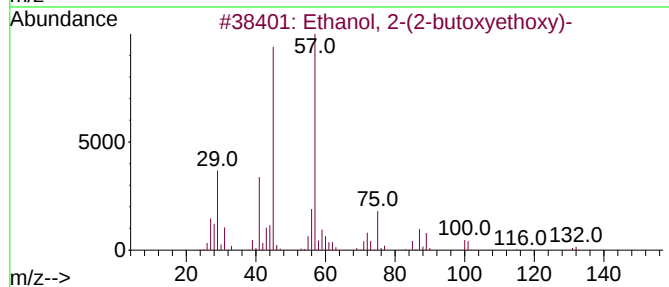
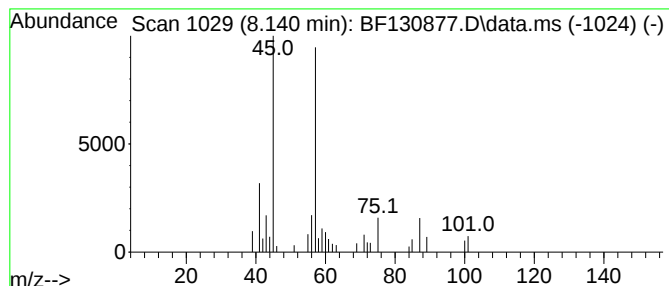
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF102722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.140	2.09 ng	68587	Naphthalene-d8	8.228

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	86
2			Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	59
3			Di-sec-Butyl ether	130	C8H18O	006863-58-7	50
4			Butane, 1,1'-[oxybis(2,1-ethaned...	218	C12H26O3	000112-73-2	50
5			2-Hexanol, 5-methyl-	116	C7H16O	000627-59-8	43



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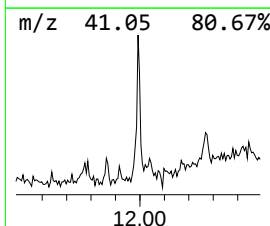
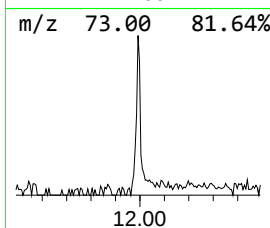
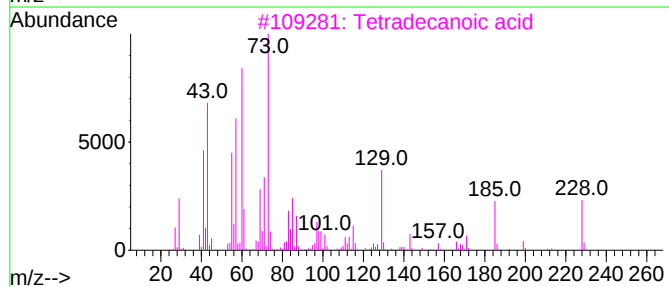
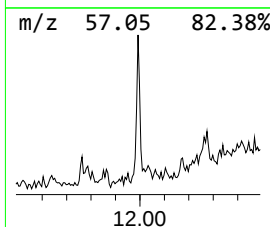
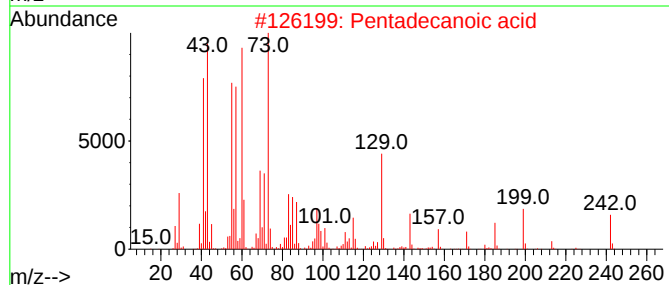
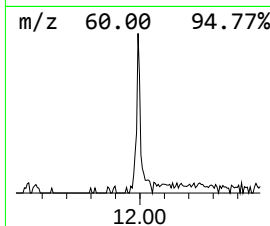
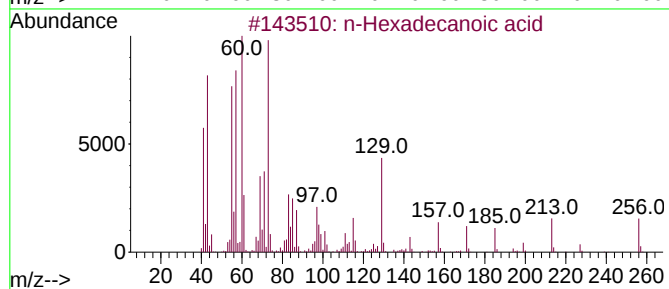
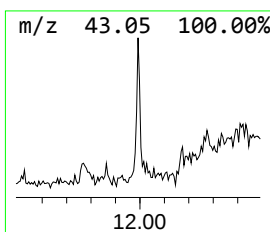
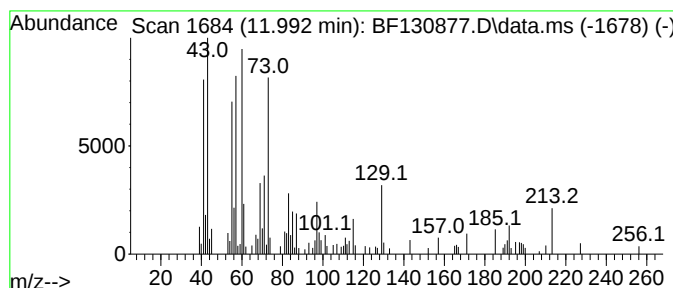
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.992	3.02 ng	111198	Phenanthrene-d10	11.480

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	72
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	68
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	68
4			Undecanoic acid	186	C11H22O2	000112-37-8	58
5			Tridecanoic acid	214	C13H26O2	000638-53-9	58



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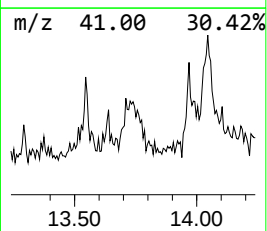
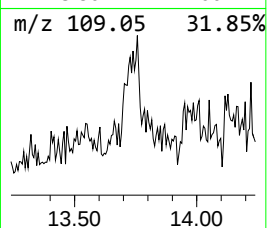
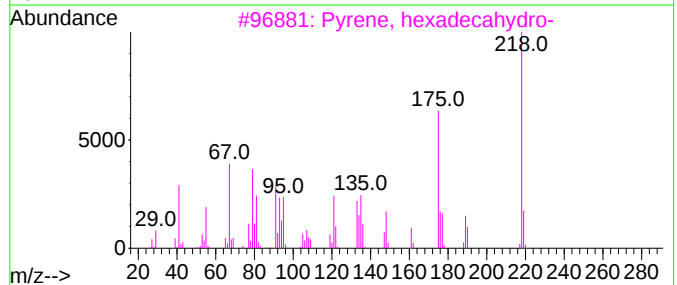
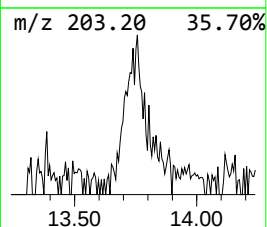
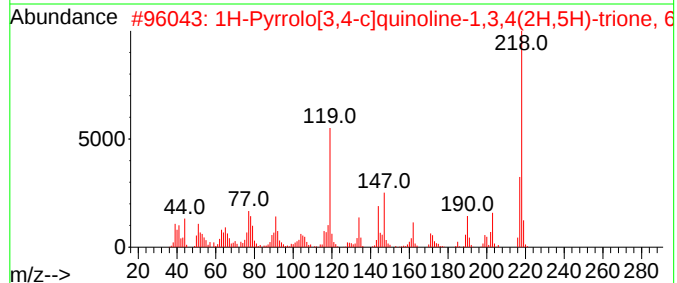
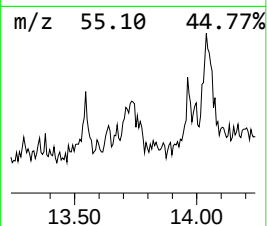
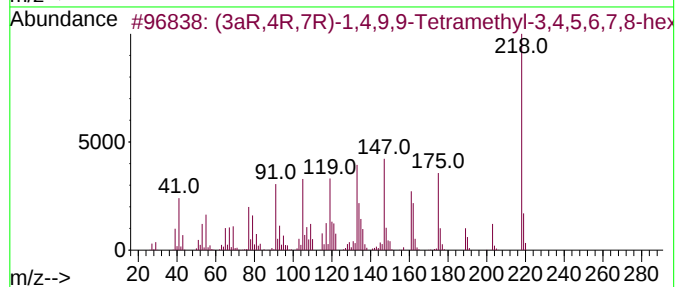
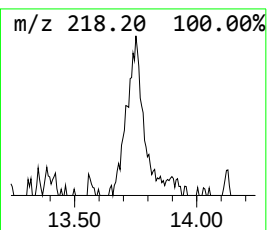
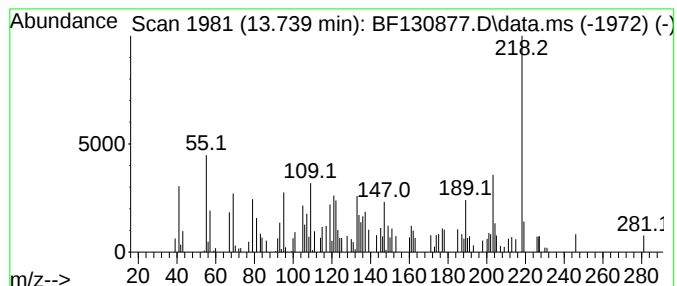
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 unknown13.739 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.739	2.79 ng	73436	Chrysene-d12	14.127

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			(3aR,4R,7R)-1,4,9,9-Tetramethyl-...	218	C15H22O	003466-15-7	49
2			1H-Pyrrolo[3,4-c]quinoline-1,3,4...	218	C11H10N2O3	181021-85-2	46
3			Pyrene, hexadecahydro-	218	C16H26	002435-85-0	46
4			3,4,6,7-Tetrahydrobenzo[1,2-b:5...	218	C12H10O4	019839-03-3	38
5			Benzo[b]naphtho[2,3-d]furan	218	C16H10O	000243-42-5	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF103122\
Data File : BF130877.D
Acq On : 31 Oct 2022 13:54
Operator : CG\JU
Sample : N5234-02
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
LSP-SS-03-03-05

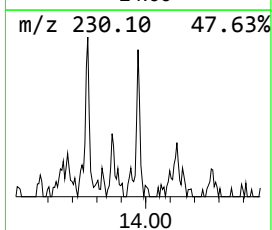
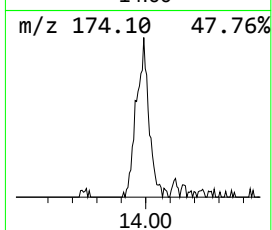
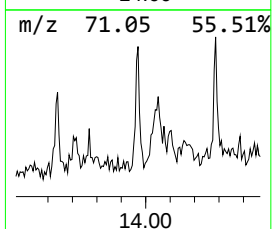
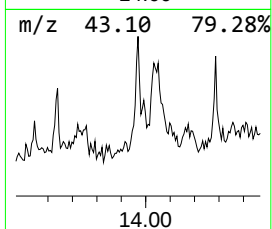
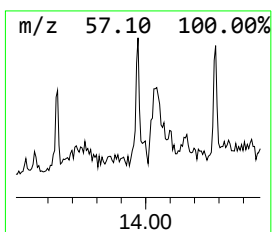
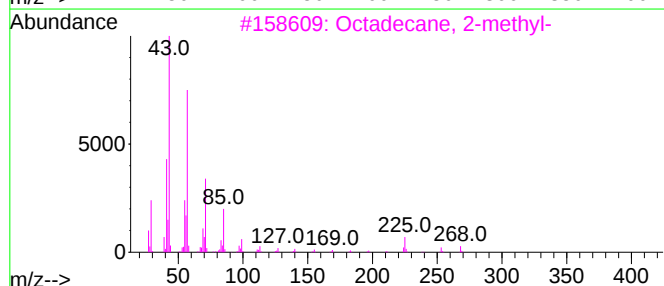
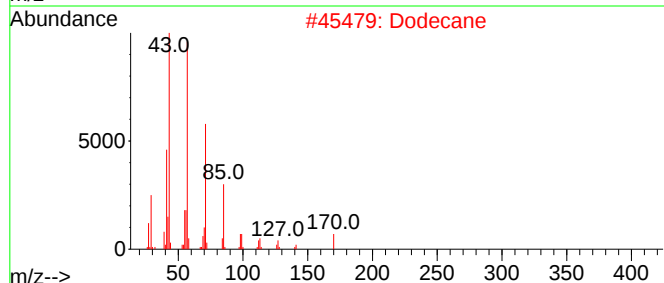
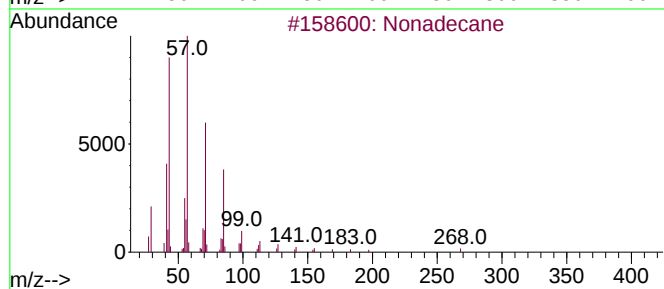
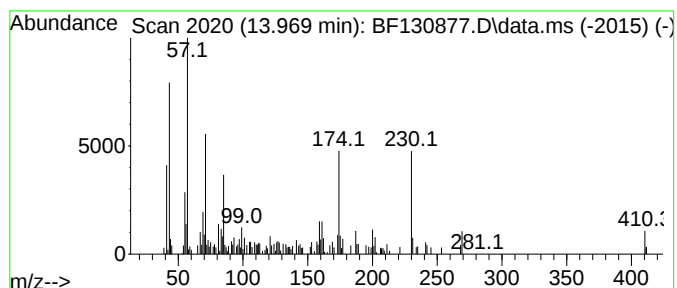
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Nonadecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.969	4.03 ng	106201	Chrysene-d12	14.127

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Nonadecane	268	C19H40	000629-92-5	51
2			Dodecane	170	C12H26	000112-40-3	35
3			Octadecane, 2-methyl-	268	C19H40	001560-88-9	25
4			Eicosane, 7-hexyl-	366	C26H54	055333-99-8	20
5			Octacosane	394	C28H58	000630-02-4	20



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF103122\
Data File : BF130877.D
Acq On : 31 Oct 2022 13:54
Operator : CG\JU
Sample : N5234-02
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
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ClientSampleId :
LSP-SS-03-03-05

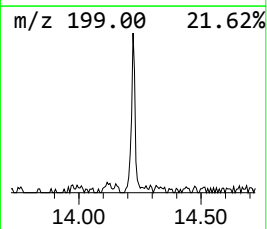
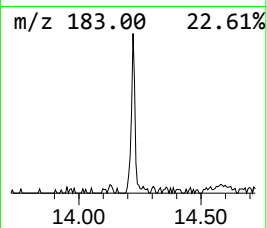
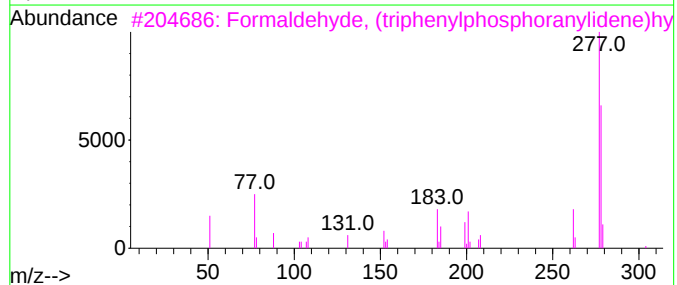
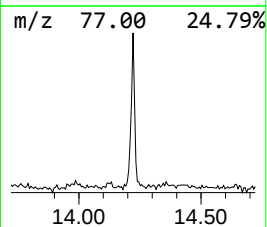
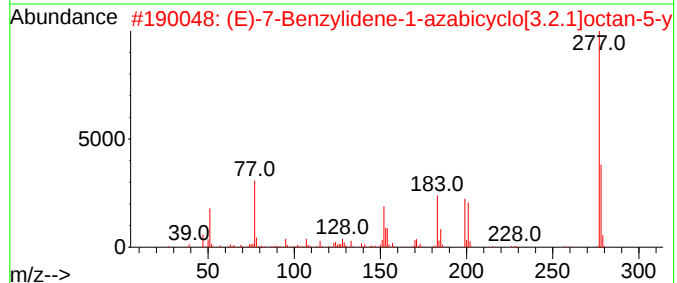
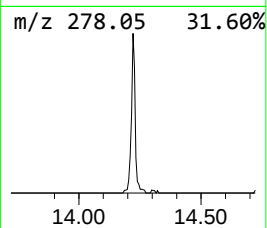
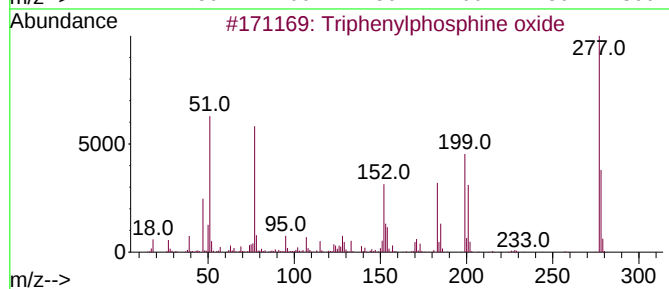
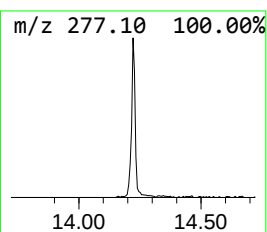
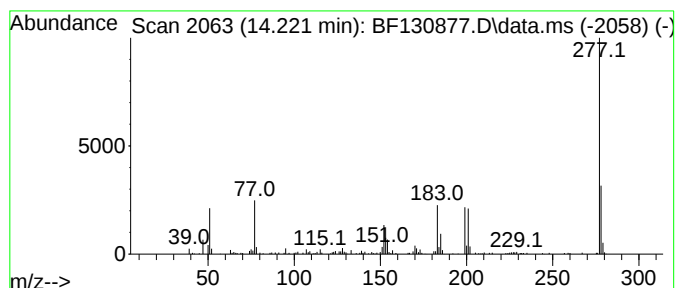
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Triphenylphosphine oxide Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.222	5.21 ng	137362	Chrysene-d12	14.127

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Triphenylphosphine oxide	278	C18H15OP	000791-28-6	97
2			(E)-7-Benzylidene-1-azabicyclo[3...]	293	C15H19N03S	1000483-83-4	58
3			Formaldehyde, (triphenylphosphor...	304	C19H17N2P	015990-54-2	50
4			Furo[3,2-c]quinoline, 8-bromo-2...	277	C13H12BrNO	1000310-92-7	38
5			Vanadium, cycloheptatrienyl-(pen...	277	C17H22V	1000155-20-5	37



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF103122\
Data File : BF130877.D
Acq On : 31 Oct 2022 13:54
Operator : CG\JU
Sample : N5234-02
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
LSP-SS-03-03-05

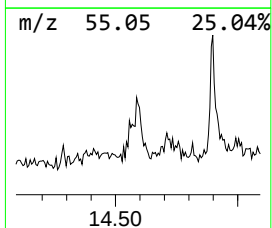
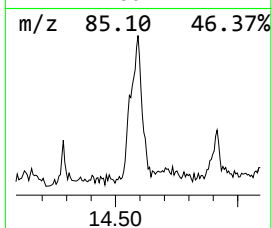
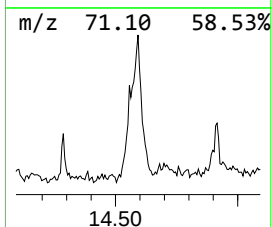
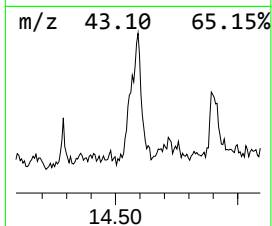
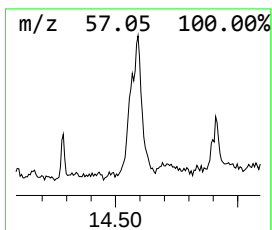
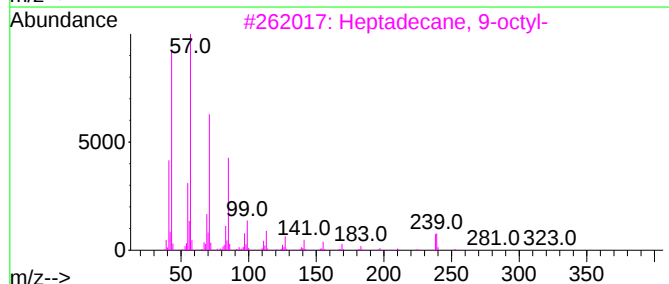
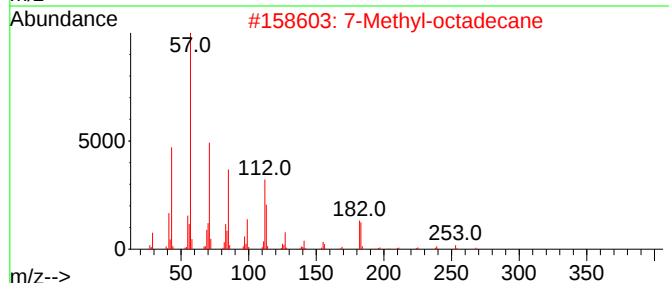
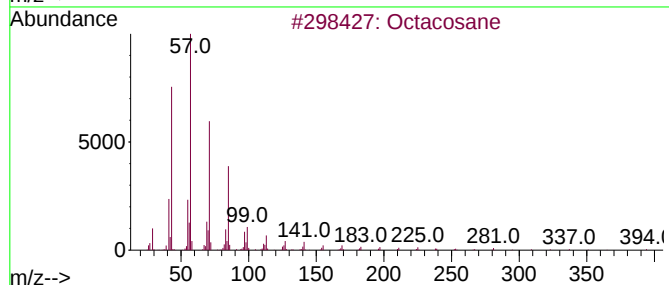
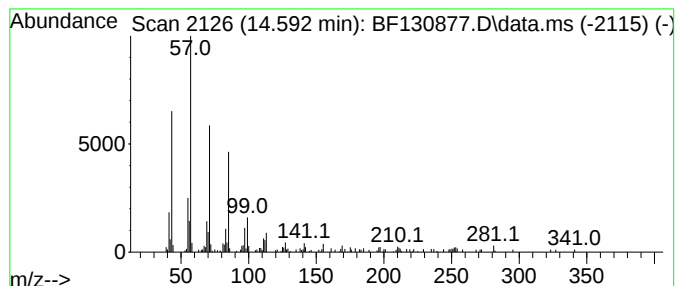
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Octacosane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.592	9.51 ng	250685	Chrysene-d12	14.127

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octacosane	394	C28H58	000630-02-4	90
2			7-Methyl-octadecane	268	C19H40	1000192-63-3	87
3			Heptadecane, 9-octyl-	352	C25H52	007225-64-1	87
4			Octacosane, 2-methyl-	408	C29H60	001560-98-1	87
5			Hentriacontane	437	C31H64	000630-04-6	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF103122\
Data File : BF130877.D
Acq On : 31 Oct 2022 13:54
Operator : CG\JU
Sample : N5234-02
Misc :
ALS Vial : 7 Sample Multiplier: 1

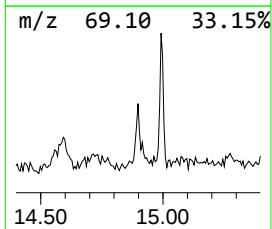
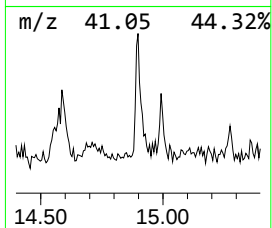
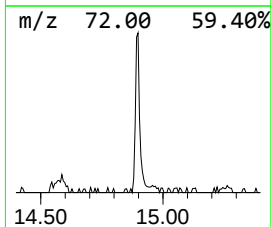
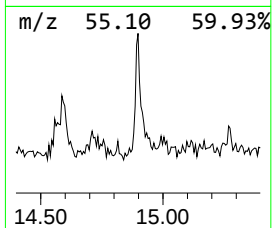
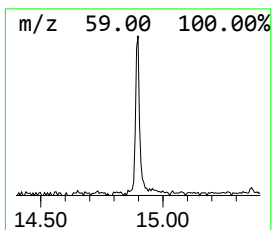
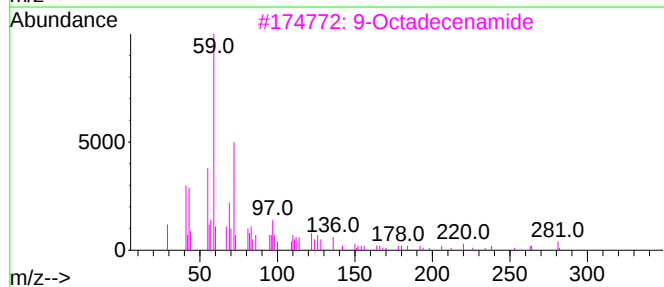
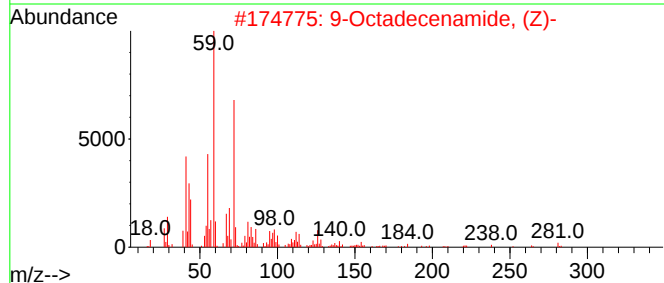
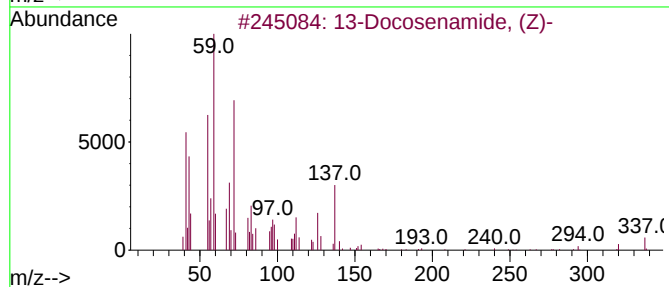
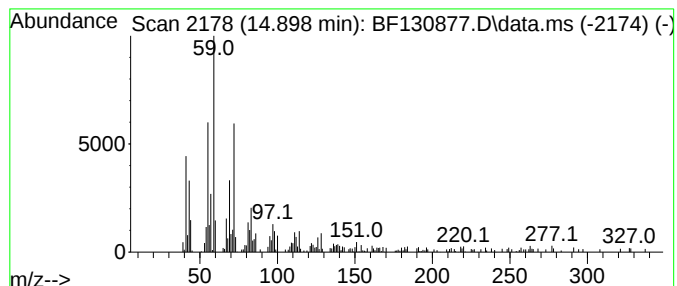
Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF102722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 13-Docosenamide, (Z)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.898	7.38 ng	165227	Perylene-d12	15.645	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	13-Docosenamide, (Z)-	337	C22H43NO	000112-84-5	83
2	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	74
3	9-Octadecenamide	281	C18H35NO	003322-62-1	64
4	Tetradecanamide	227	C14H29NO	000638-58-4	46
5	Benzeneethanamine, 2-fluoro-.bet...	229	C11H16FN03	061338-98-5	43



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF103122\
Data File : BF130877.D
Acq On : 31 Oct 2022 13:54
Operator : CG\JU
Sample : N5234-02
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
LSP-SS-03-03-05

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
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2-Pentanone, 4-...	5.169	14.0	ng	359019	1	6.940	514281	20.0
Ethanol, 2-(2-b...	8.140	2.1	ng	68587	2	8.228	657290	20.0
n-Hexadecanoic ...	11.992	3.0	ng	111198	4	11.480	736307	20.0
unknown13.739	13.739	2.8	ng	73436	5	14.127	527110	20.0
Nonadecane	13.969	4.0	ng	106201	5	14.127	527110	20.0
Triphenylphosph...	14.222	5.2	ng	137362	5	14.127	527110	20.0
Octacosane	14.592	9.5	ng	250685	5	14.127	527110	20.0
13-Docosenamide...	14.898	7.4	ng	165227	6	15.645	447992	20.0