

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF020224\
 Data File : BF137265.D
 Acq On : 02 Feb 2024 20:16
 Operator : CG\JU
 Sample : P1341-02
 Misc :
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 COMP-2

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-BF013024.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF137265.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.110	3	4	10	rVB	110239	99850	4.72%	0.679%
2	5.040	498	502	510	rVB	39211	49554	2.34%	0.337%
3	5.428	564	568	582	rBV	1551282	1627616	76.87%	11.070%
4	6.428	733	738	759	rBV	1547970	1617773	76.40%	11.004%
5	6.792	796	800	807	rBV	342991	318979	15.06%	2.170%
6	7.351	890	895	898	rBV	1113310	987546	46.64%	6.717%
7	8.069	1013	1017	1020	rBV	438183	394867	18.65%	2.686%
8	9.145	1196	1200	1203	rBV	2145842	1815984	85.77%	12.352%
9	9.822	1311	1315	1319	rBV	529884	410971	19.41%	2.795%
10	10.610	1445	1449	1458	rBV	1059758	984884	46.51%	6.699%
11	10.986	1505	1513	1518	rBV	10901	33554	1.58%	0.228%
12	11.310	1565	1568	1571	rBV	409162	374200	17.67%	2.545%
13	11.333	1571	1572	1578	rVB	64561	50429	2.38%	0.343%
14	11.786	1644	1649	1652	rBV	15878	29510	1.39%	0.201%
15	11.857	1657	1661	1664	rBV2	104608	132139	6.24%	0.899%
16	11.886	1664	1666	1670	rVB	22897	26307	1.24%	0.179%
17	12.527	1772	1775	1778	rBV	126378	112301	5.30%	0.764%
18	12.645	1792	1795	1805	rVB4	33036	53794	2.54%	0.366%
19	12.757	1809	1814	1818	rVV	95312	93260	4.40%	0.634%
20	12.910	1836	1840	1844	rBV	1794450	1722745	81.36%	11.718%
21	13.092	1864	1871	1875	rBV2	14060	27919	1.32%	0.190%
22	13.157	1878	1882	1885	rBV4	19747	22557	1.07%	0.153%
23	13.392	1919	1922	1926	rBV	92513	78629	3.71%	0.535%
24	13.486	1935	1938	1946	rBV	280494	248527	11.74%	1.690%
25	13.710	1973	1976	1979	rBV3	28005	29400	1.39%	0.200%
26	13.774	1983	1987	1991	rBV3	24964	32653	1.54%	0.222%
27	13.810	1991	1993	1995	rBV	26311	27855	1.32%	0.189%
28	13.845	1997	1999	2012	rVB2	41918	81773	3.86%	0.556%
29	13.963	2015	2019	2023	rBV	2239969	2117366	100.00%	14.402%
30	14.174	2053	2055	2058	rVB	34038	28592	1.35%	0.194%
31	14.304	2074	2077	2080	rBV	26290	26088	1.23%	0.177%
32	14.457	2101	2103	2106	rBV2	30687	34425	1.63%	0.234%
33	14.533	2114	2116	2117	rBV2	31242	25447	1.20%	0.173%
34	14.557	2117	2120	2126	rVB	52699	89810	4.24%	0.611%
35	14.615	2126	2130	2135	rBV	467693	446206	21.07%	3.035%
36	14.745	2149	2152	2155	rBV	64576	80708	3.81%	0.549%

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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-BF013024.M
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37	15.115	2213	2215	2220	rVB2	47695	54093	2.55%	0.368%
38	15.445	2267	2271	2275	rBV	175962	217553	10.27%	1.480%
39	15.510	2280	2282	2291	rVB3	30429	52841	2.50%	0.359%
40	15.968	2356	2360	2364	rBV2	28309	43610	2.06%	0.297%

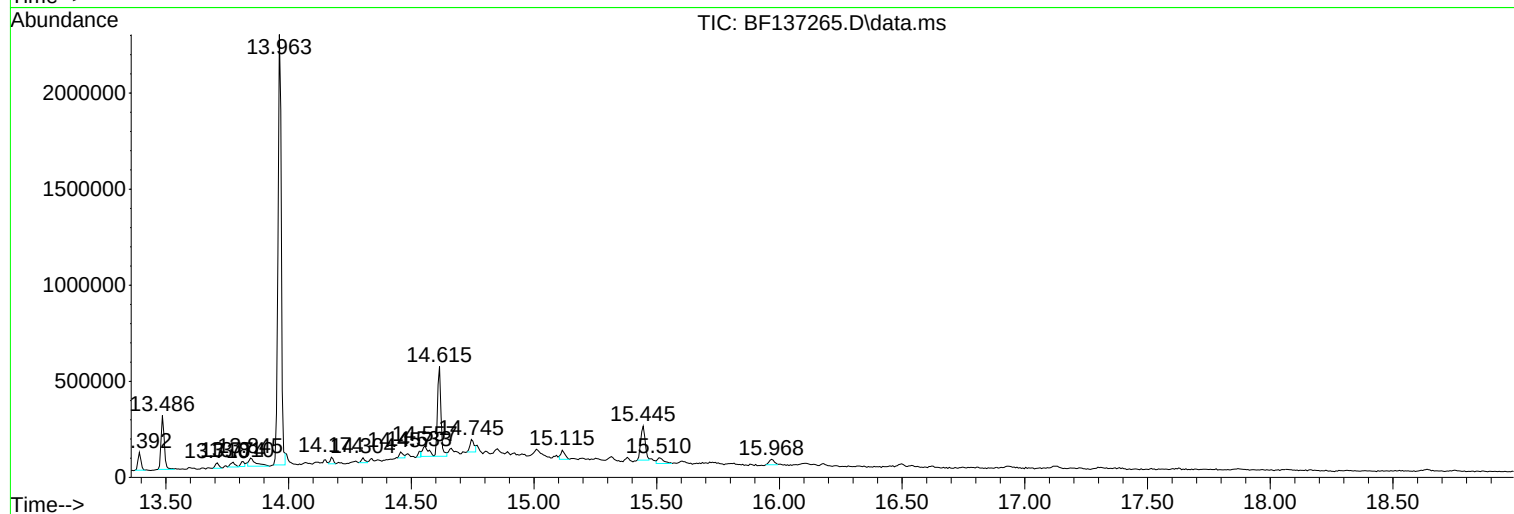
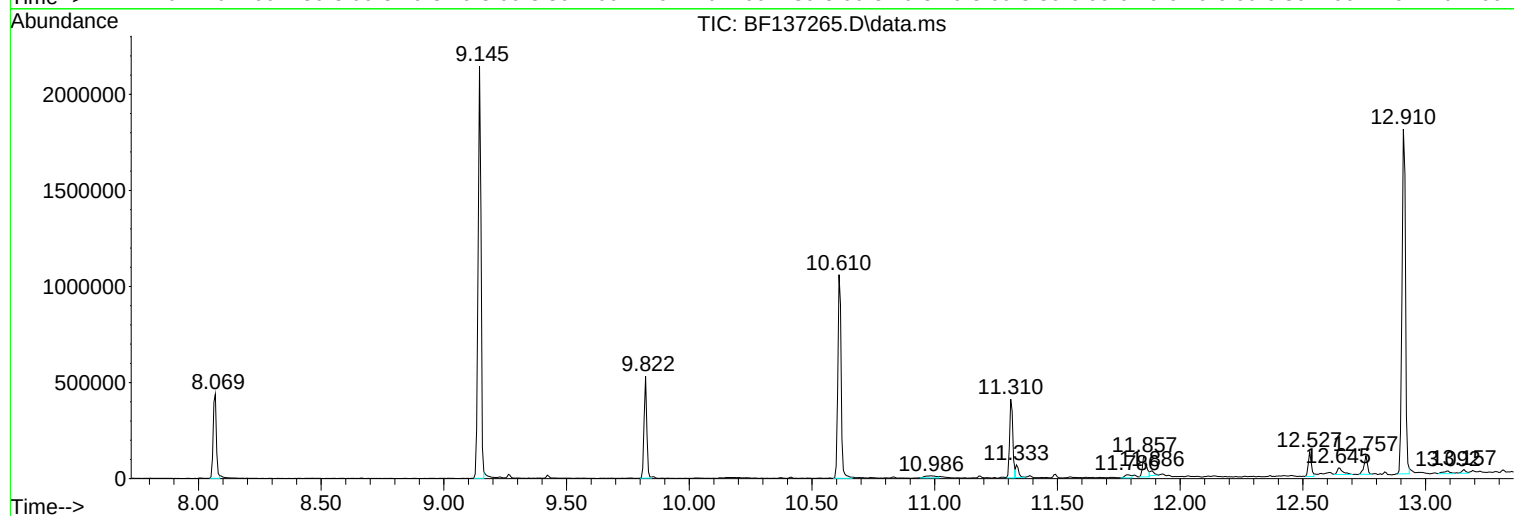
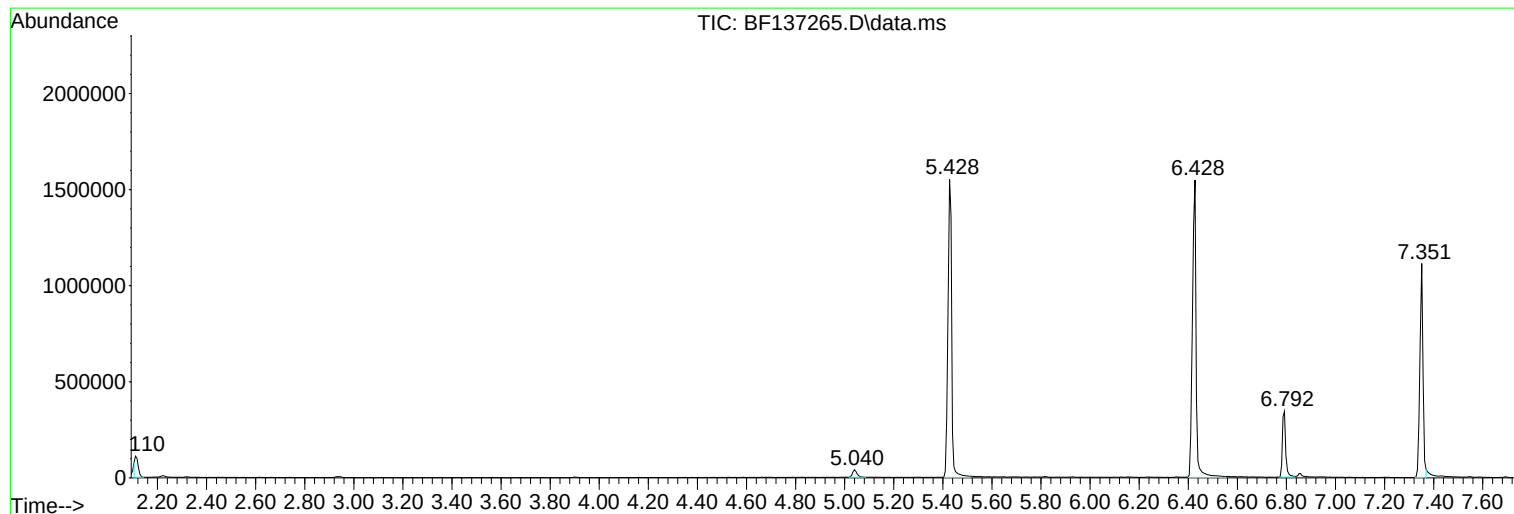
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF013024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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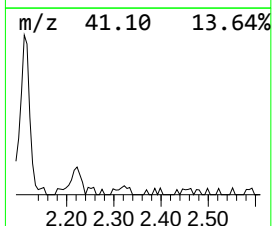
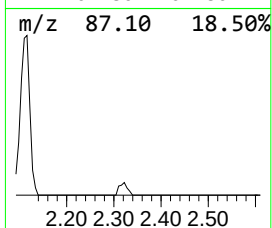
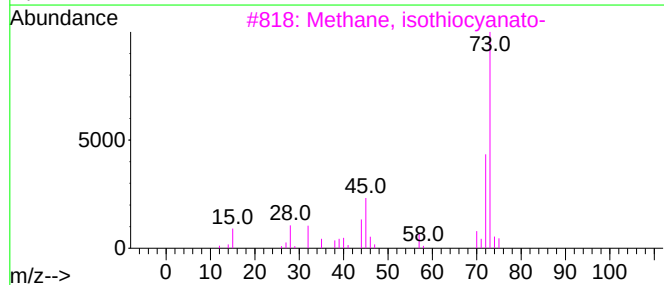
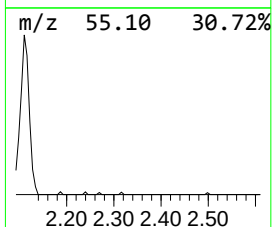
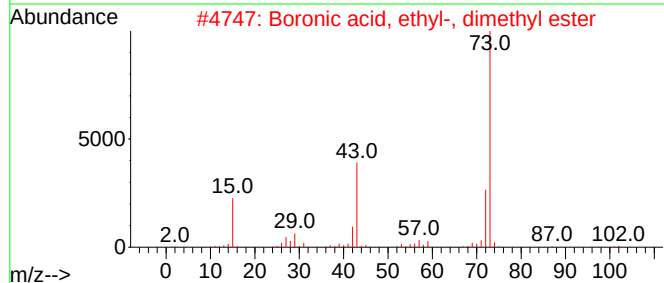
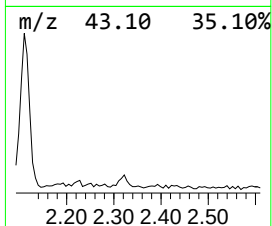
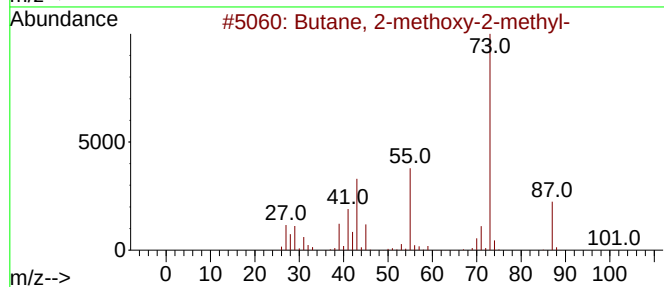
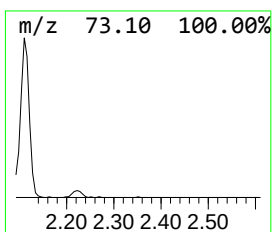
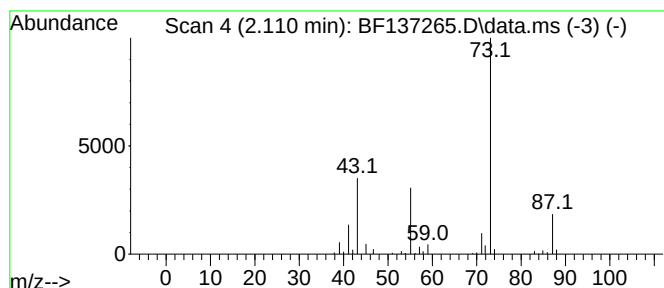
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF013024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 unknown2.110 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.110	6.26 ng	99850	1,4-Dichlorobenzene-d4	6.792

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	38
2			Boronic acid, ethyl-, dimethyl e...	102	C4H11BO2	007318-82-3	9
3			Methane, isothiocyanato-	73	C2H3NS	000556-61-6	7
4			Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	5
5			Thiocyanic acid, ethyl ester	87	C3H5NS	000542-90-5	5



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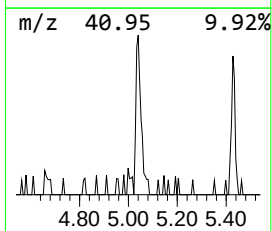
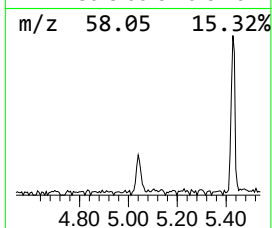
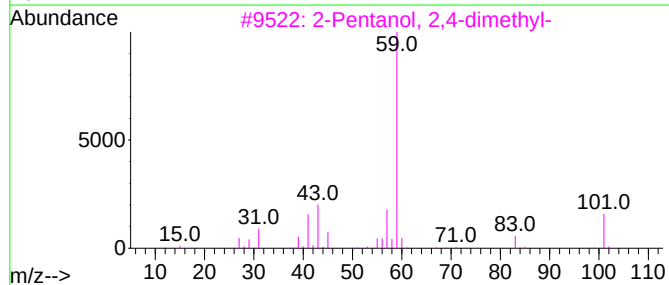
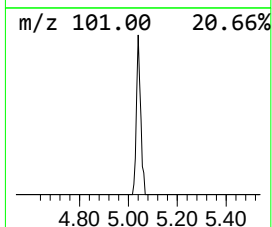
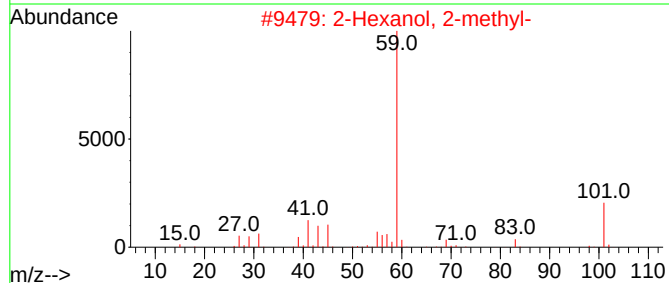
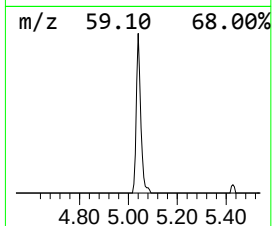
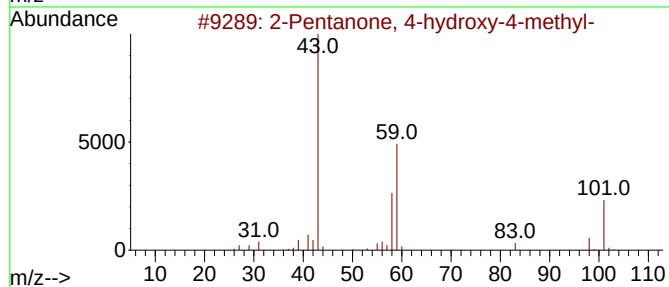
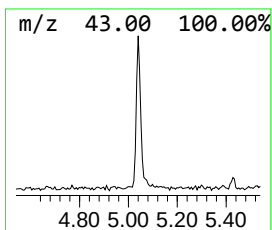
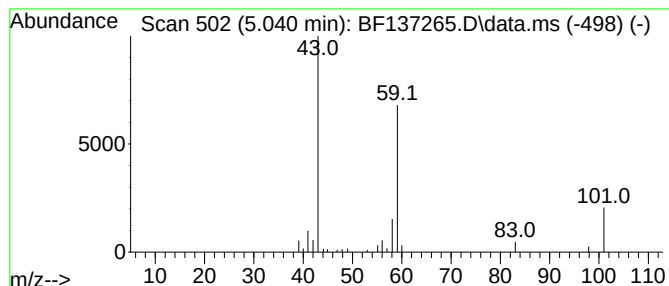
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD			R.T.
5.040	3.11 ng	49554	1,4-Dichlorobenzene-d4			6.792
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-		116	C6H12O2	000123-42-2	64
2	2-Hexanol, 2-methyl-		116	C7H16O	000625-23-0	33
3	2-Pentanol, 2,4-dimethyl-		116	C7H16O	000625-06-9	25
4	1,8-Nonanediol, 8-methyl-		174	C10H22O2	054725-73-4	23
5	1,2-Butanediol		90	C4H10O2	000584-03-2	23



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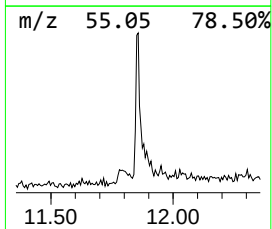
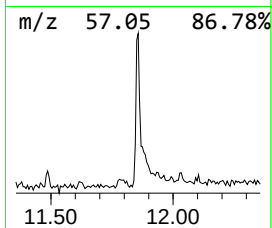
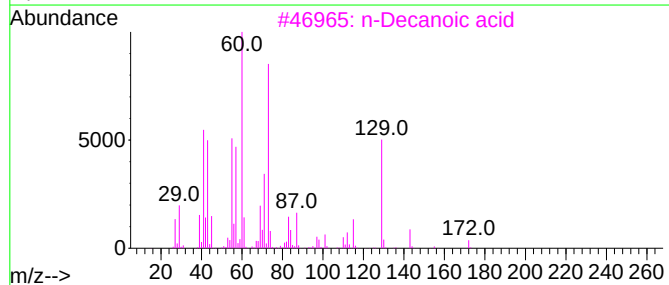
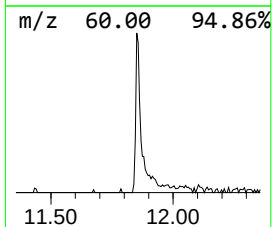
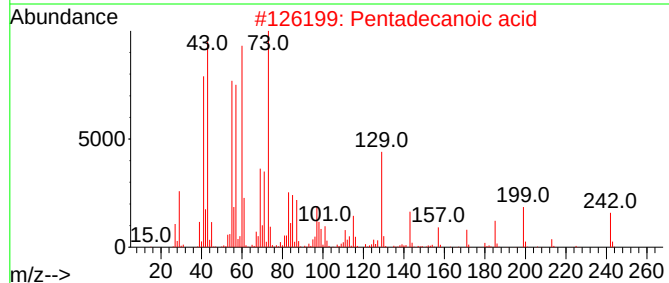
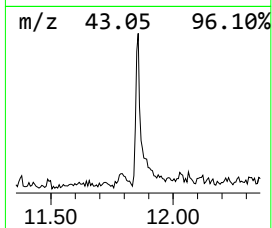
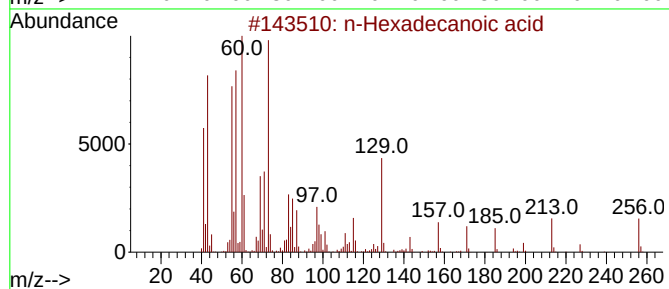
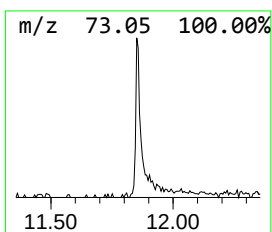
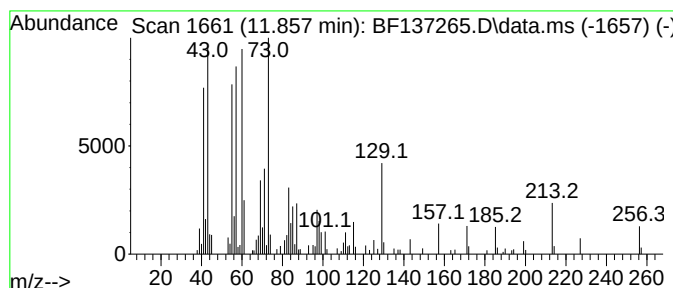
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.857	7.06 ng	132139	Phenanthrene-d10	11.310

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		n-Decanoic acid	172	C10H20O2	000334-48-5	86
4		Tetradecanoic acid	228	C14H28O2	000544-63-8	86
5		Tridecanoic acid	214	C13H26O2	000638-53-9	74



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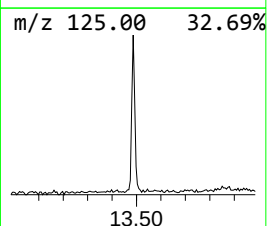
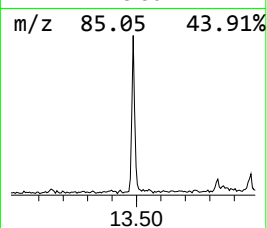
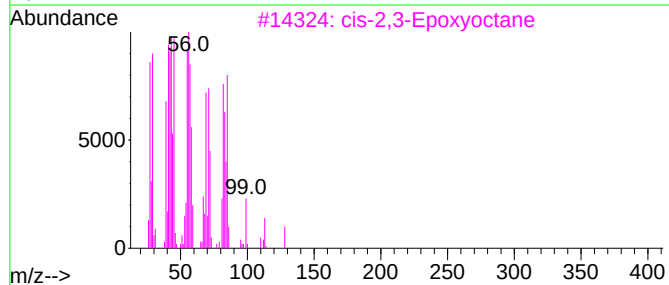
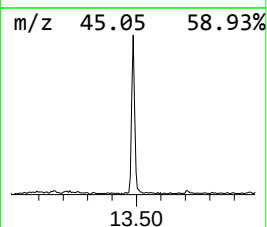
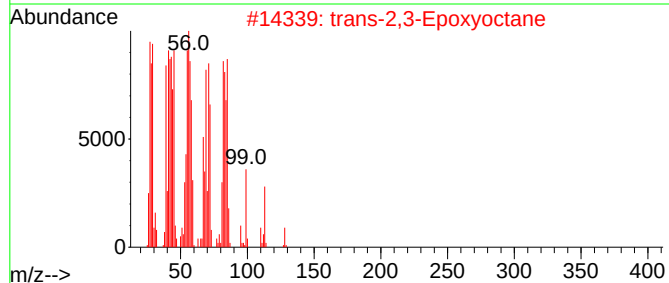
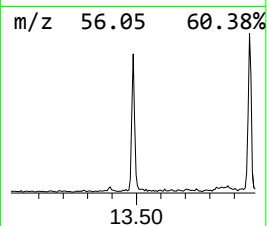
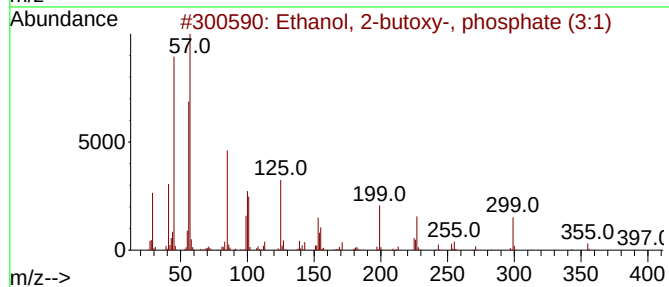
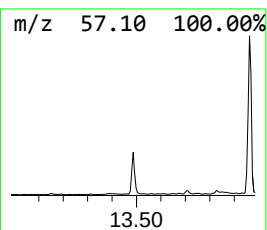
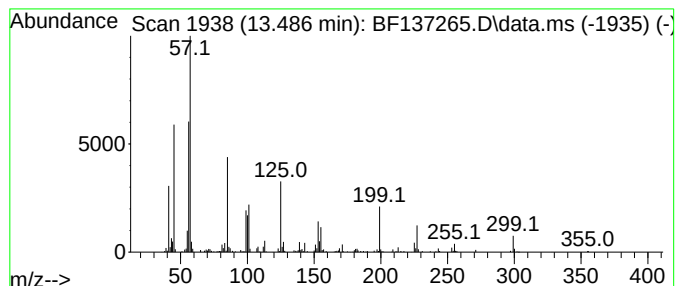
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Ethanol, 2-butoxy-, phospho... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.486	2.35 ng	248527	Chrysene-d12	13.963

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-butoxy-, phosphate (3:1)	398	C18H39O7P	000078-51-3	83
2			trans-2,3-Epoxyoctane	128	C8H16O	028180-70-3	47
3			cis-2,3-Epoxyoctane	128	C8H16O	023024-54-6	38
4			Butane, 1,1'-[oxybis(2,1-ethaned...	218	C12H26O3	000112-73-2	16
5			Butane, 2,2,3-trimethyl-	100	C7H16	000464-06-2	12



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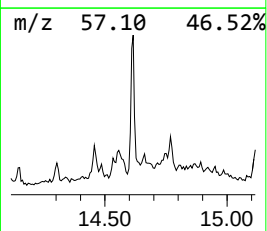
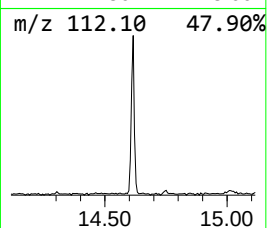
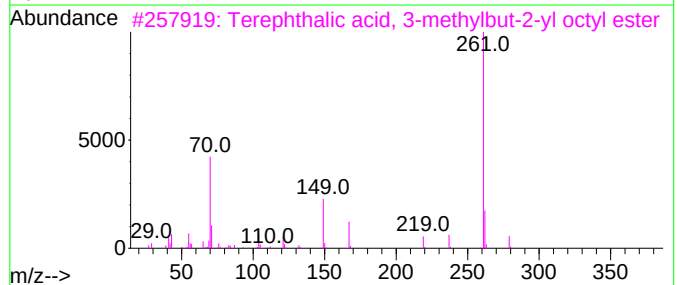
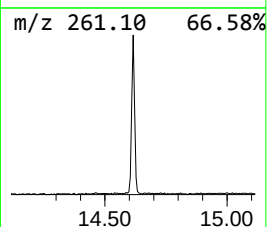
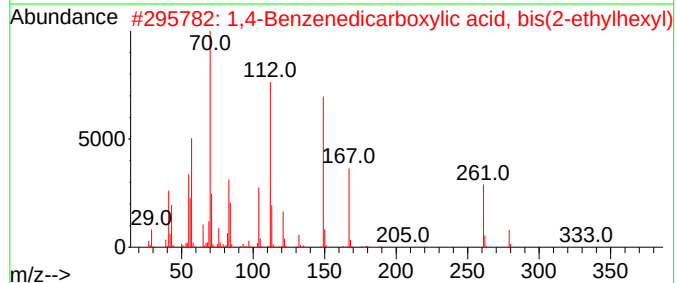
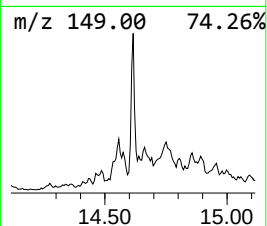
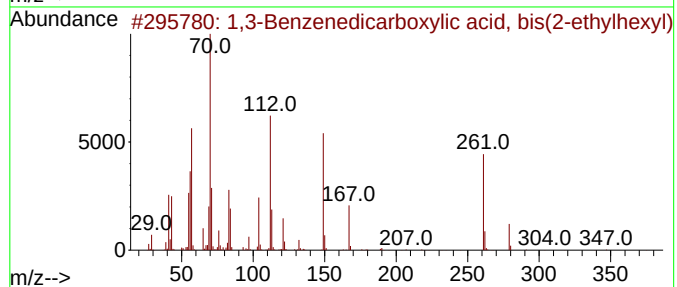
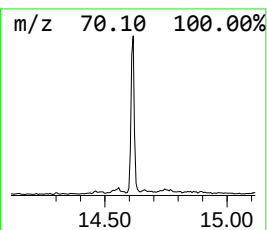
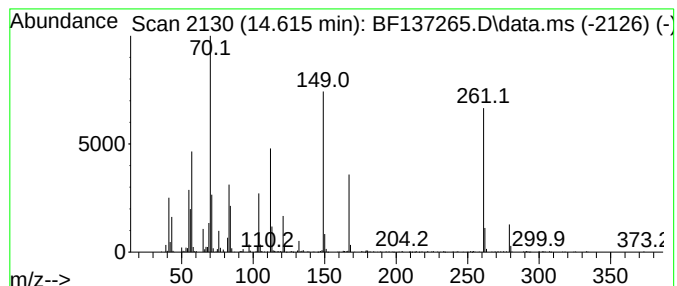
Instrument :
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 1,3-Benzenedicarboxylic aci... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.615	4.21 ng	446206	Chrysene-d12	13.963	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3-Benzenedicarboxylic acid, bi...	390	C24H38O4	000137-89-3	80
2	1,4-Benzenedicarboxylic acid, bi...	390	C24H38O4	006422-86-2	58
3	Terephthalic acid, 3-methylbut-2...	348	C21H32O4	1000356-27-6	52
4	Terephthalic acid, 2-ethylhexyl ...	390	C24H38O4	1000324-00-5	49
5	Isophthalic acid, 3-methylbut-2-...	348	C21H32O4	1000344-72-4	47



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF020224\
Data File : BF137265.D
Acq On : 02 Feb 2024 20:16
Operator : CG\JU
Sample : P1341-02
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
COMP-2

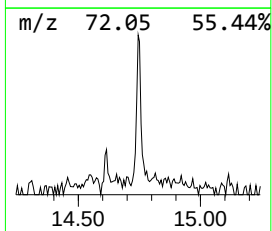
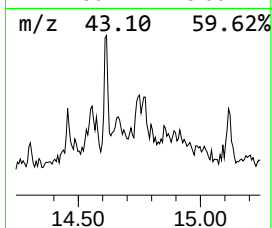
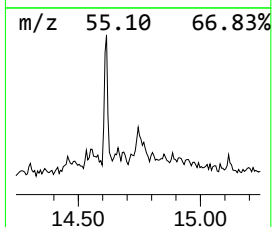
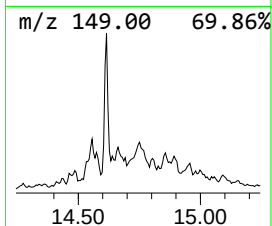
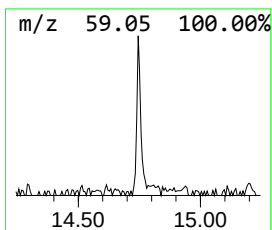
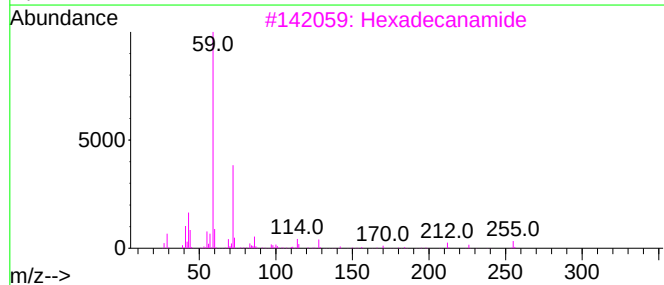
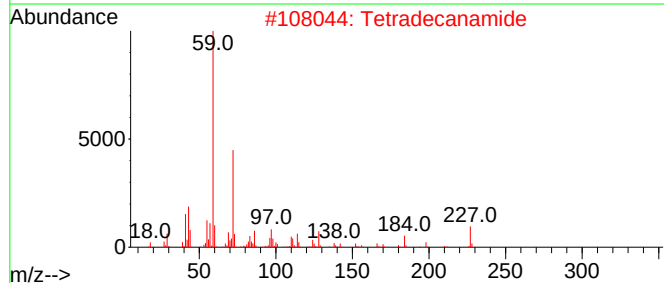
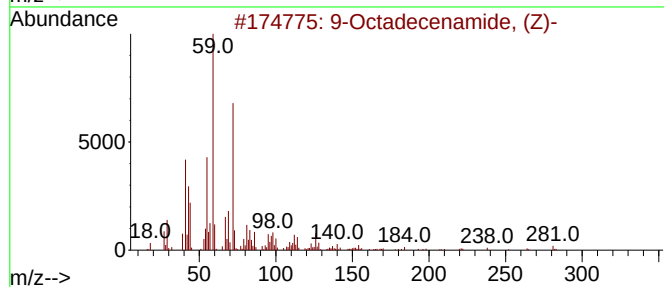
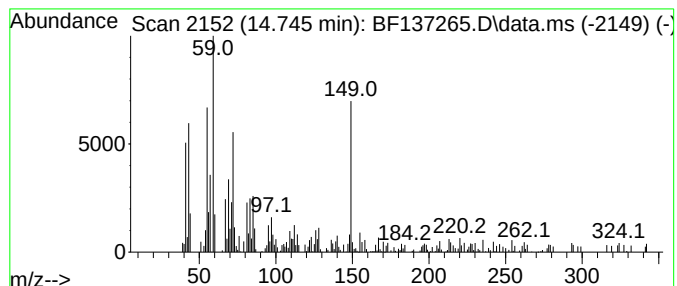
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 9-Octadecenamide, (Z)- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.745	7.42 ng	80708	Perylene-d12	15.445

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	95	
2	Tetradecanamide	227	C14H29NO	000638-58-4	70	
3	Hexadecanamide	255	C16H33NO	000629-54-9	49	
4	9-Octadecenamide	281	C18H35NO	003322-62-1	49	
5	Octadecanamide	283	C18H37NO	000124-26-5	47	



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF020224\
Data File : BF137265.D
Acq On : 02 Feb 2024 20:16
Operator : CG\JU
Sample : P1341-02
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
COMP-2

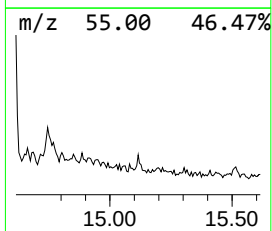
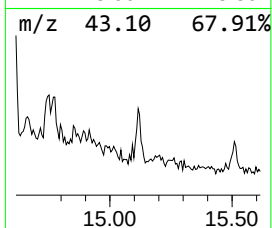
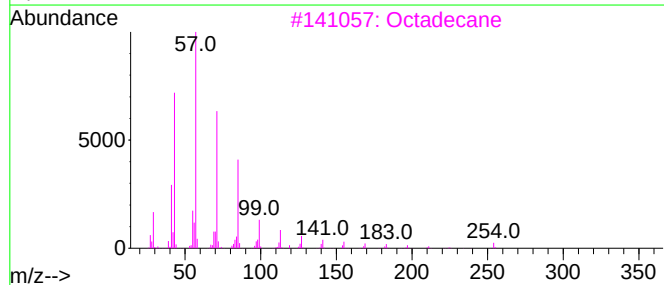
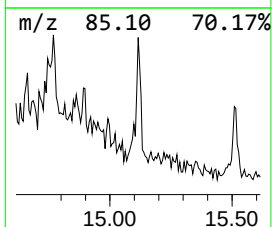
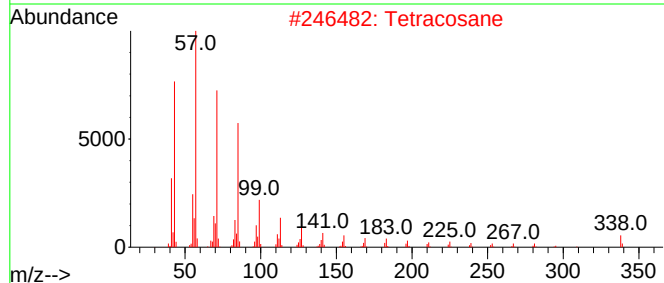
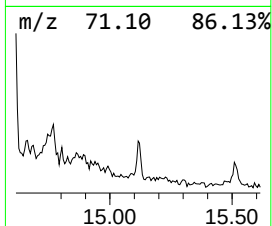
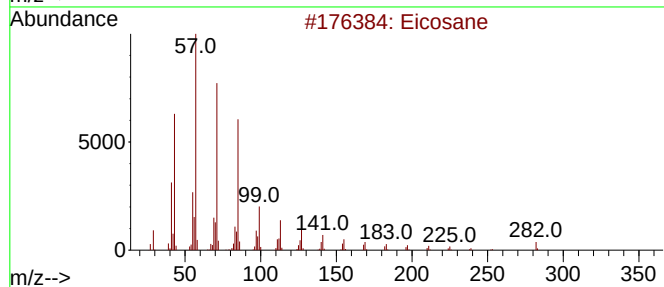
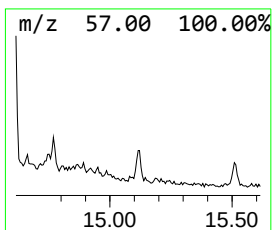
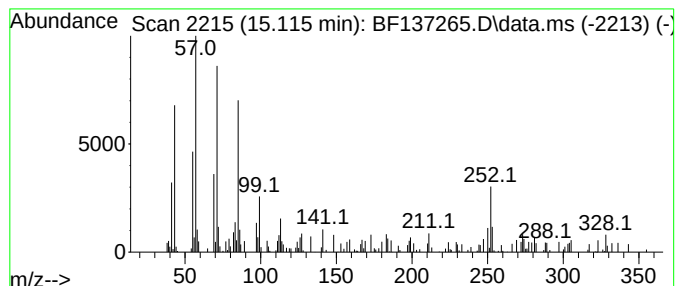
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Eicosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.115	4.97 ng	54093	Perylene-d12	15.445

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Eicosane	282	C20H42	000112-95-8	93
2			Tetracosane	338	C24H50	000646-31-1	58
3			Octadecane	254	C18H38	000593-45-3	58
4			Tetracosane, 1-iodo-	464	C24H49I	1000406-32-0	58
5			Pentacosane	352	C25H52	000629-99-2	58



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF020224\
Data File : BF137265.D
Acq On : 02 Feb 2024 20:16
Operator : CG\JU
Sample : P1341-02
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
COMP-2

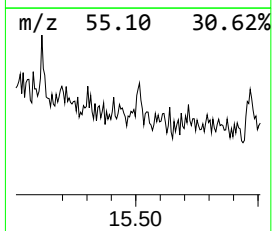
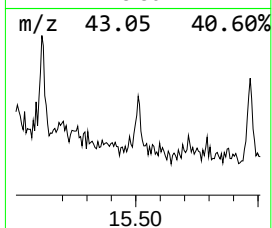
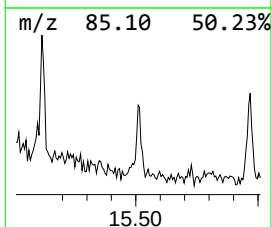
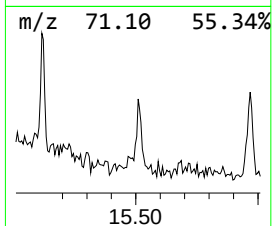
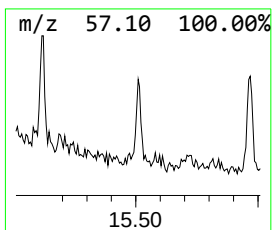
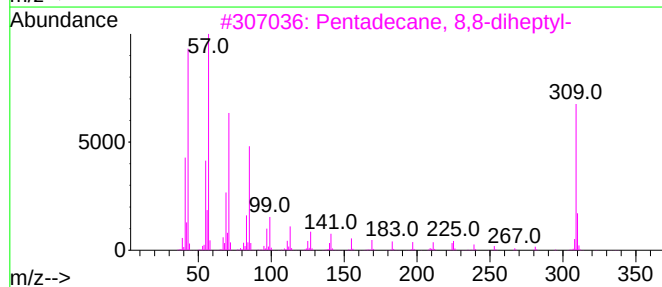
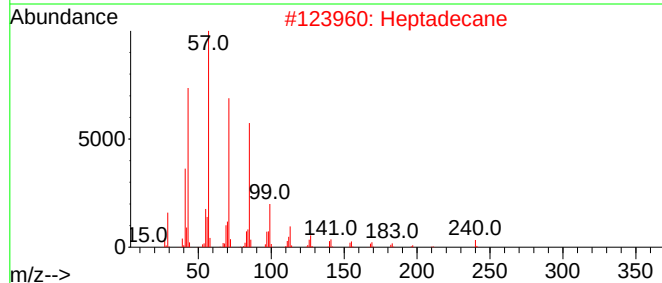
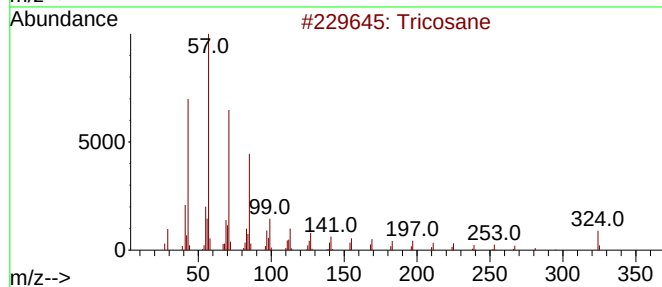
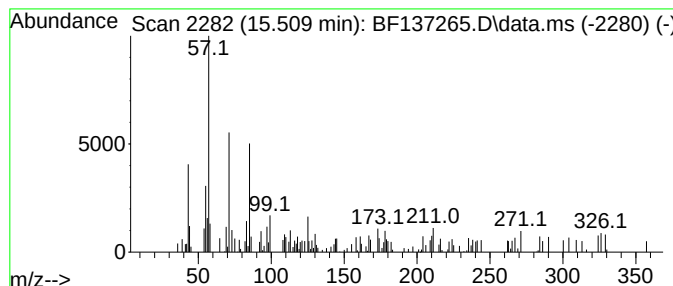
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Tricosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.509	4.86 ng	52841	Perylene-d12	15.445

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tricosane	324	C23H48	000638-67-5	64
2			Heptadecane	240	C17H36	000629-78-7	60
3			Pentadecane, 8,8-diheptyl-	408	C29H60	055268-72-9	50
4			Hentriacontane	437	C31H64	000630-04-6	50
5			Sulfurous acid, butyl octadecyl ...	390	C22H46O3S	1000309-18-5	47



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF020224\
Data File : BF137265.D
Acq On : 02 Feb 2024 20:16
Operator : CG\JU
Sample : P1341-02
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
COMP-2

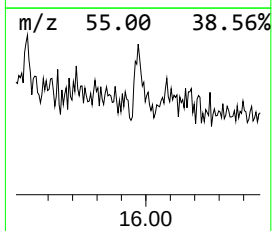
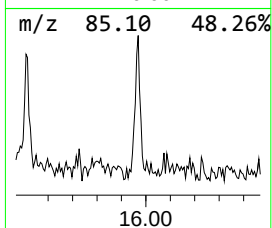
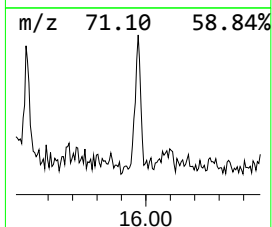
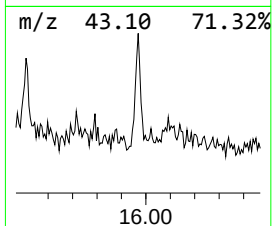
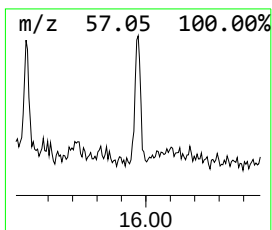
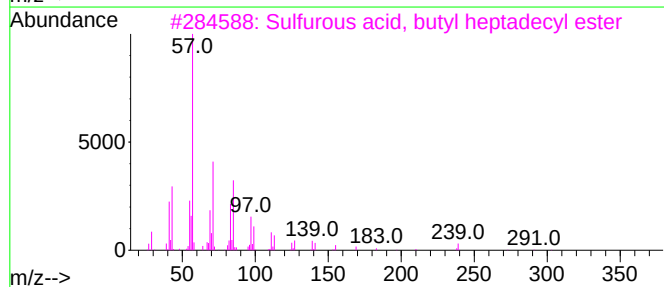
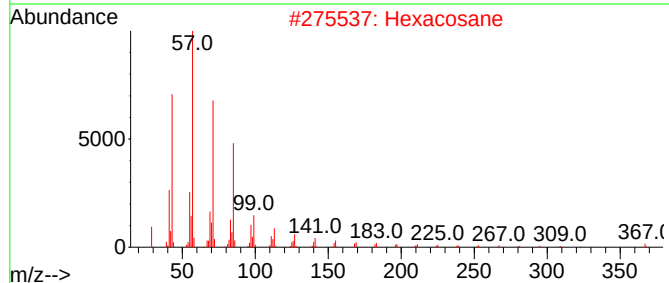
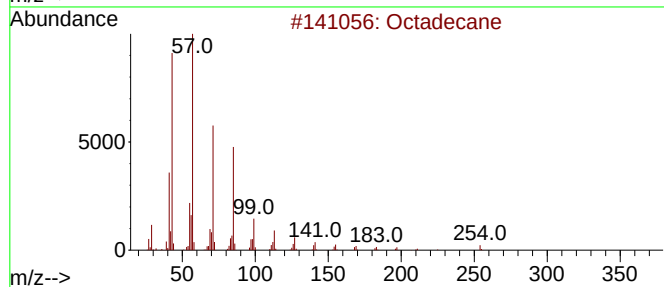
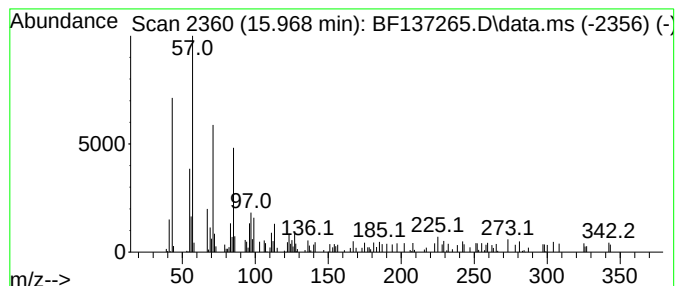
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Octadecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.968	4.01 ng	43610	Perylene-d12	15.445

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecane	254	C18H38	000593-45-3	58
2			Hexacosane	366	C26H54	000630-01-3	58
3			Sulfurous acid, butyl heptadecyl...	376	C21H44O3S	1000309-18-4	58
4			Eicosane, 2-methyl-	296	C21H44	001560-84-5	58
5			Heneicosane	296	C21H44	000629-94-7	58



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF020224\
Data File : BF137265.D
Acq On : 02 Feb 2024 20:16
Operator : CG\JU
Sample : P1341-02
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
COMP-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF013024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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					#	RT	Resp	Conc
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n-Hexadecanoic ...	11.857	7.1	ng	132139	4	11.310	374200	20.0
Ethanol, 2-buto...	13.486	2.4	ng	248527	5	13.963	2117370	20.0
1,3-Benzenedica...	14.615	4.2	ng	446206	5	13.963	2117370	20.0
9-Octadecenamid...	14.745	7.4	ng	80708	6	15.445	217553	20.0
Eicosane	15.115	5.0	ng	54093	6	15.445	217553	20.0
Tricosane	15.509	4.9	ng	52841	6	15.445	217553	20.0
Octadecane	15.968	4.0	ng	43610	6	15.445	217553	20.0