

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF070122\
 Data File : BF129088.D
 Acq On : 01 Jul 2022 12:56
 Operator : CG\JU
 Sample : N3543-01
 Misc :
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 KENS-062822-SB18-GW

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-BF062922.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF129088.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.322	3	6	12	rVB	6306726	7993630	68.67%	10.453%
2	4.104	305	309	316	rVB	114757	143746	1.23%	0.188%
3	5.581	555	560	563	rBV	4928315	4357347	37.43%	5.698%
4	6.569	724	728	738	rBV	2995221	2694145	23.14%	3.523%
5	6.951	790	793	797	rBV	2303143	2124587	18.25%	2.778%
6	7.522	883	890	893	rBV	5984938	6416106	55.12%	8.390%
7	8.239	1007	1012	1015	rBV	3200144	2874444	24.69%	3.759%
8	9.316	1189	1195	1198	rBV	11734051	11641233	100.00%	15.223%
9	9.998	1305	1311	1314	rBV	3835915	3226774	27.72%	4.220%
10	10.375	1368	1375	1378	rBV	1940181	1571011	13.50%	2.054%
11	10.610	1409	1415	1425	rBV2	60402	182416	1.57%	0.239%
12	10.792	1439	1446	1449	rBV	7590194	7278847	62.53%	9.519%
13	11.492	1560	1565	1568	rBV	3518428	3286333	28.23%	4.298%
14	11.998	1645	1651	1656	rBV	353612	471692	4.05%	0.617%
15	12.151	1673	1677	1683	rBV2	109014	142090	1.22%	0.186%
16	12.227	1683	1690	1705	rVB9	82931	291626	2.51%	0.381%
17	12.375	1708	1715	1723	rBV	119290	291387	2.50%	0.381%
18	12.786	1779	1785	1795	rVB	339763	568045	4.88%	0.743%
19	12.880	1798	1801	1807	rBV	390850	320193	2.75%	0.419%
20	13.080	1830	1835	1838	rBV	10628167	10736692	92.23%	14.040%
21	13.410	1885	1891	1903	rVB	331527	594747	5.11%	0.778%
22	14.139	2006	2015	2018	rBV	2718196	2990806	25.69%	3.911%
23	14.233	2026	2031	2036	rBV	342979	377126	3.24%	0.493%
24	14.692	2104	2109	2114	rVV	457533	709171	6.09%	0.927%
25	14.751	2116	2119	2127	rVB4	156168	250774	2.15%	0.328%
26	15.292	2205	2211	2217	rVB	266732	498884	4.29%	0.652%
27	15.663	2268	2274	2286	rVB	1573384	2008246	17.25%	2.626%
28	15.974	2323	2327	2334	rVB	113094	214537	1.84%	0.281%
29	16.498	2406	2416	2443	rBV6	334016	2213524	19.01%	2.895%

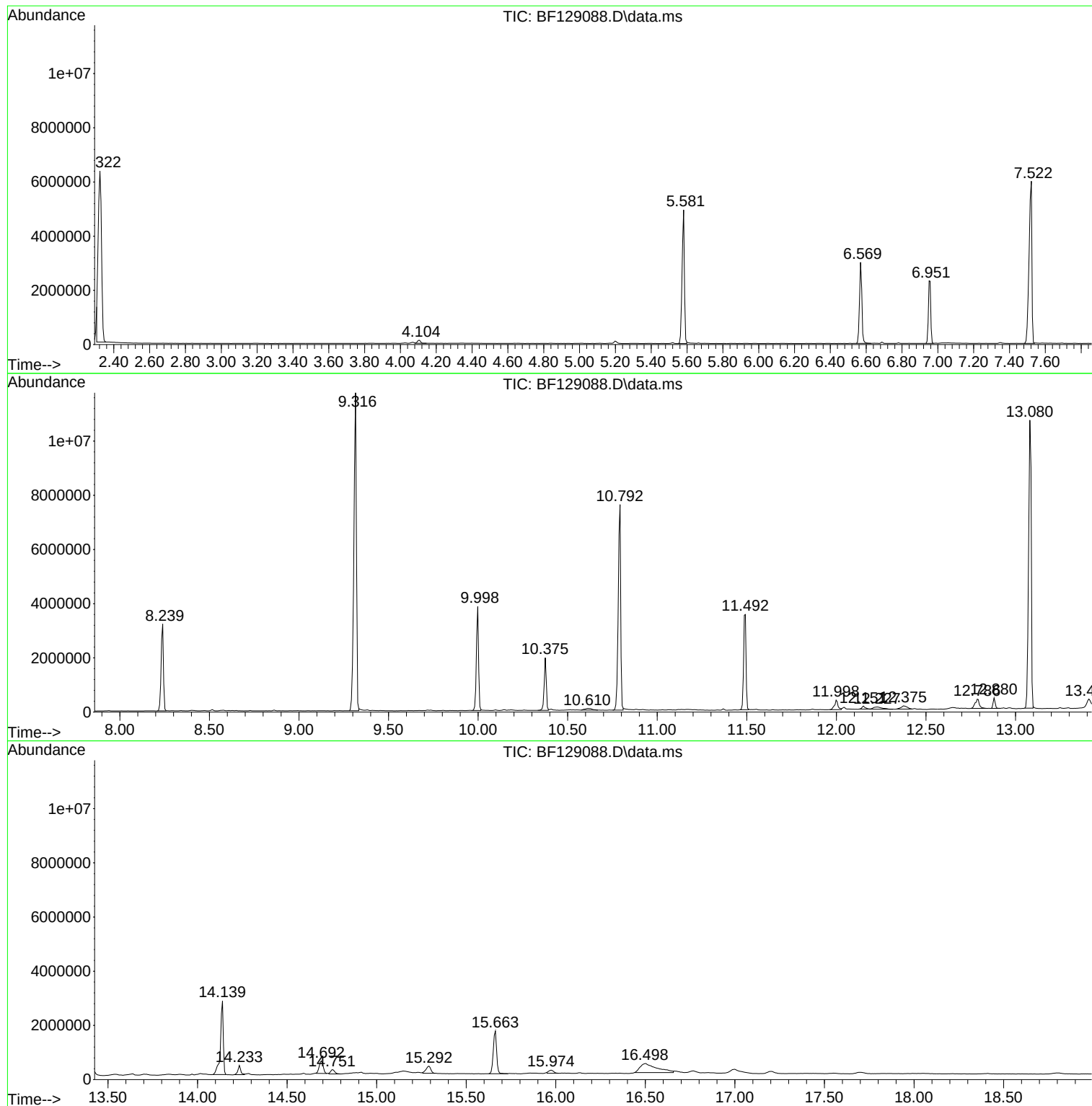
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062922.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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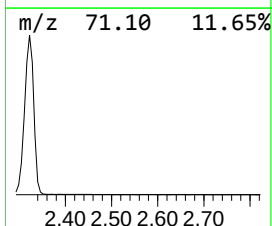
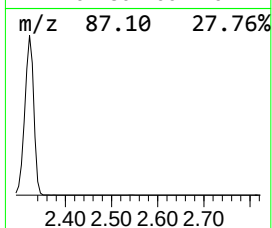
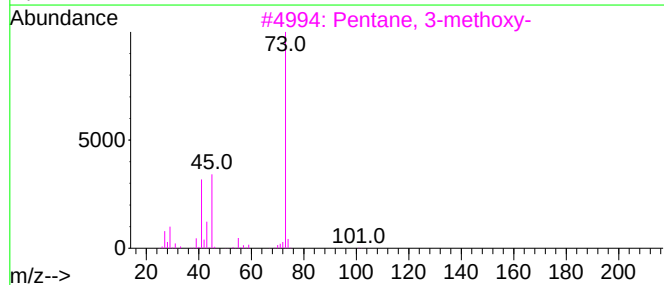
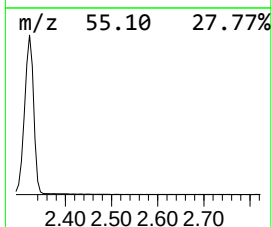
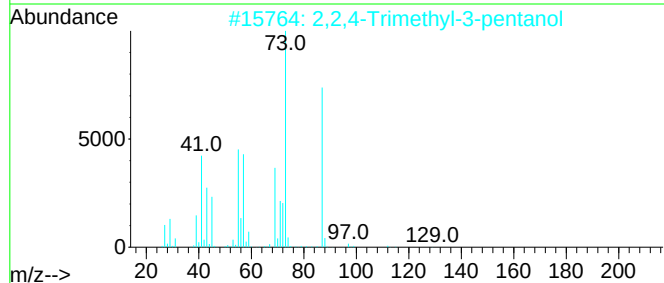
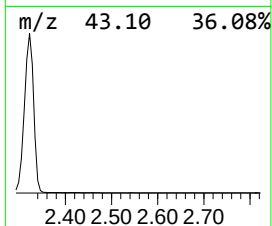
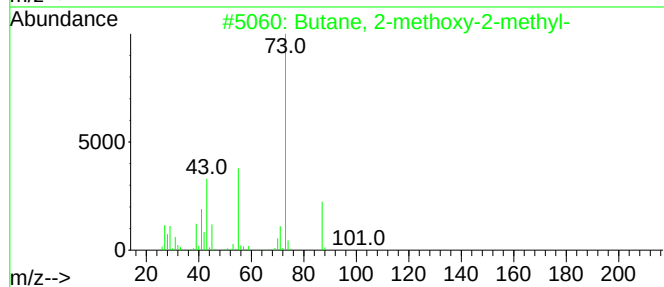
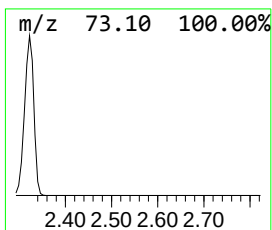
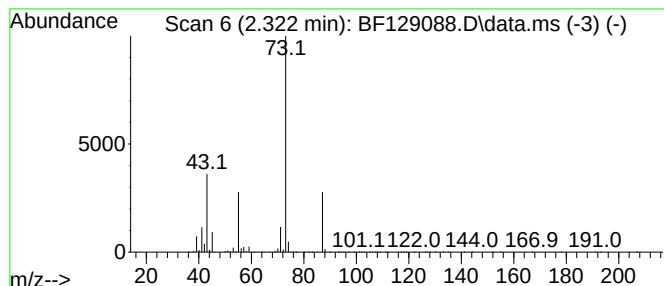
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.322	75.25 ng	7993630	1,4-Dichlorobenzene-d4	6.957

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17
4			Silane, tetramethyl-	88	C4H12Si	000075-76-3	12
5			N-Ethylformamide	73	C3H7NO	000627-45-2	9



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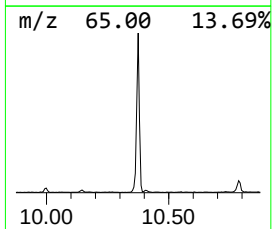
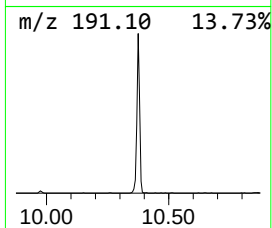
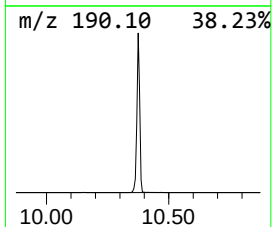
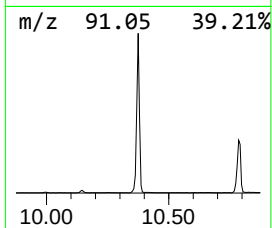
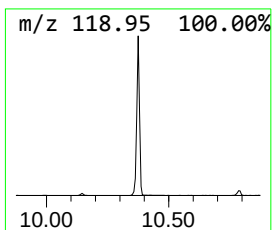
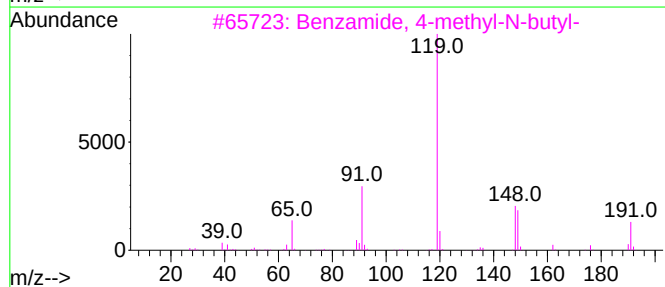
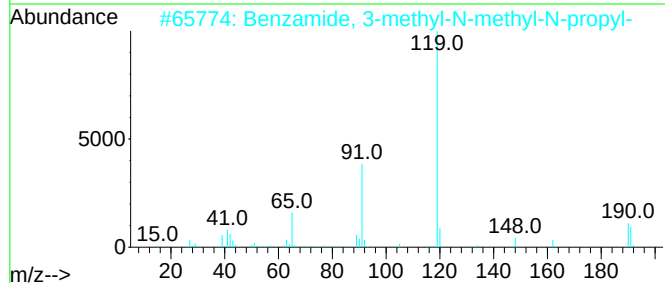
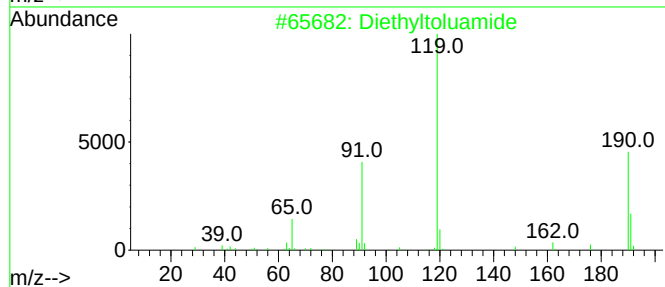
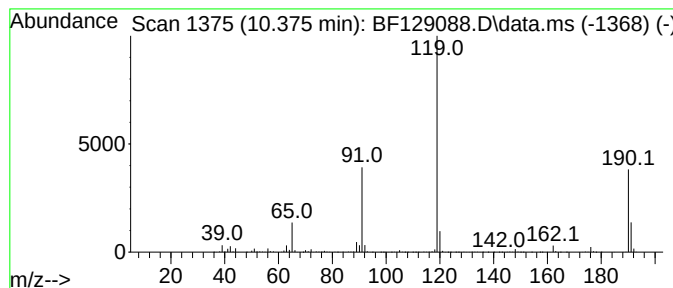
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TIC Integration Parameters: LSCINT.P

Peak Number 2 Diethyltoluamide Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.375	9.74 ng	1571010	Acenaphthene-d10	9.998

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Diethyltoluamide	191	C12H17NO	000134-62-3	97
2			Benzamide, 3-methyl-N-methyl-N-p...	191	C12H17NO	1000421-46-2	81
3			Benzamide, 4-methyl-N-butyl-	191	C12H17NO	1000407-46-6	76
4			Benzamide, 3-methyl-N-butyl-	191	C12H17NO	1000407-41-1	76
5			Benzamide, 2-methyl-N-methyl-N-p...	191	C12H17NO	1000421-44-4	74



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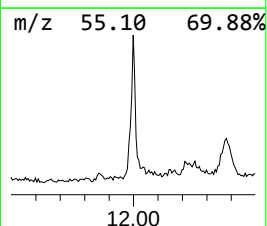
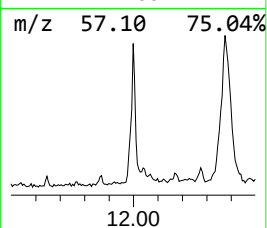
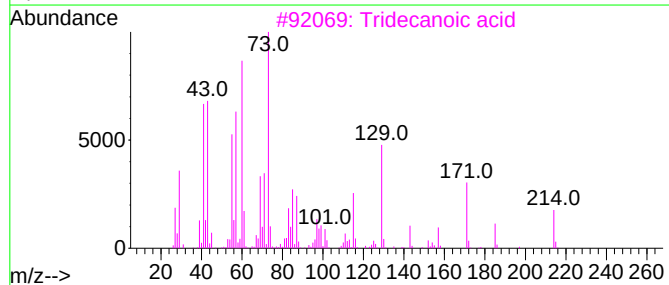
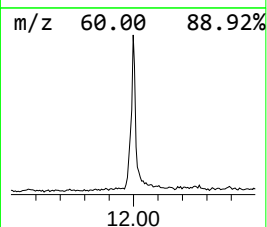
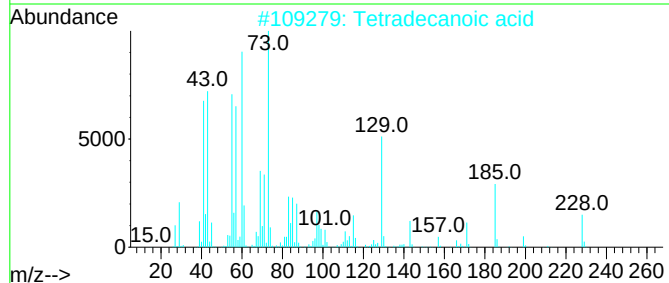
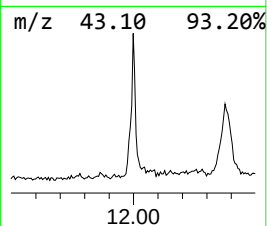
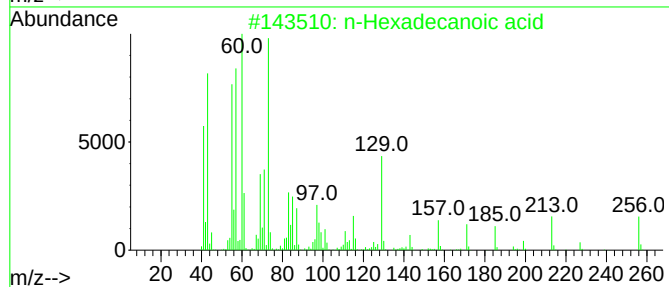
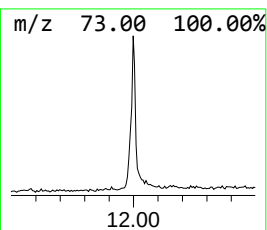
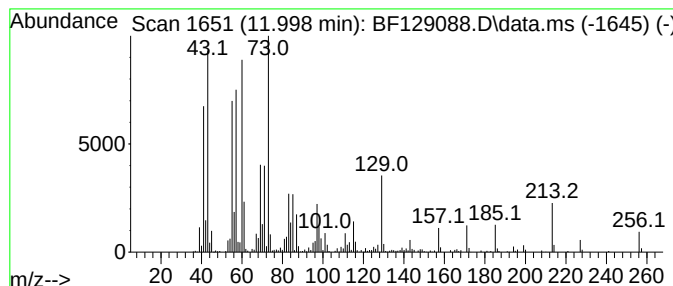
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Peak Number 3 n-Hexadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.998	2.87 ng	471692	Phenanthrene-d10	11.492

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Tetradecanoic acid	228	C14H28O2	000544-63-8	93
3			Tridecanoic acid	214	C13H26O2	000638-53-9	92
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	87
5			Octanoic acid	144	C8H16O2	000124-07-2	45



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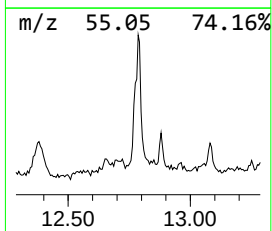
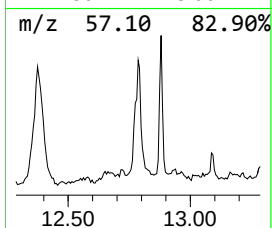
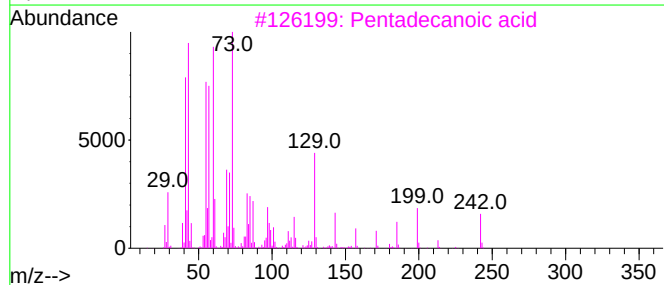
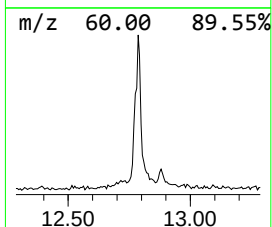
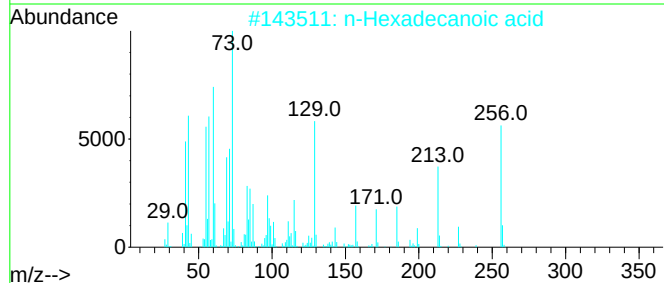
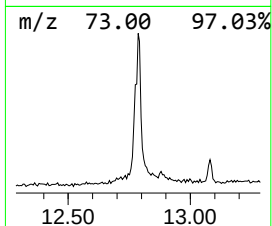
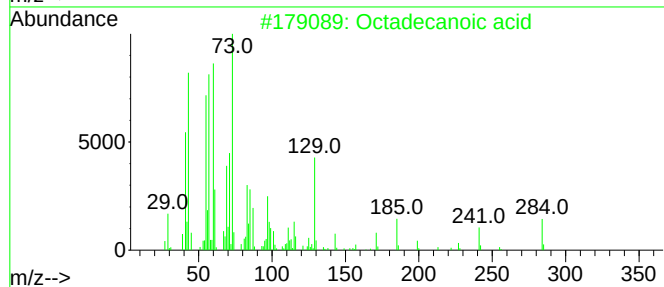
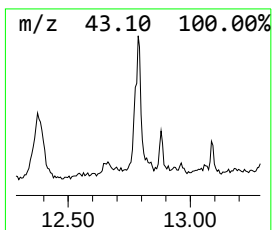
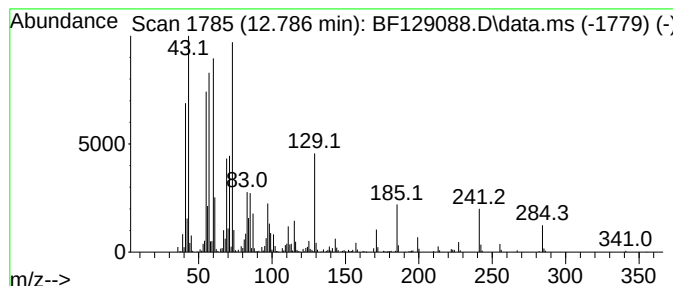
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Peak Number 4 Octadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.786	3.46 ng	568045	Phenanthrene-d10	11.492

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	99
2			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	93
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	89
4			n-Decanoic acid	172	C10H20O2	000334-48-5	64
5			Tetradecanoic acid	228	C14H28O2	000544-63-8	64



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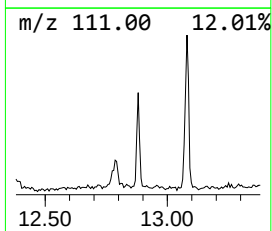
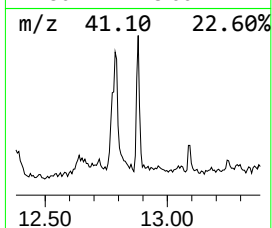
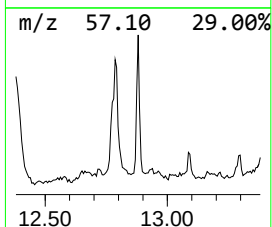
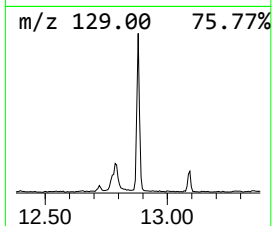
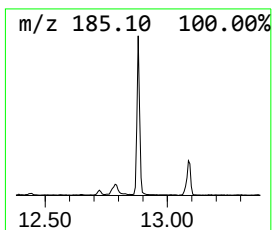
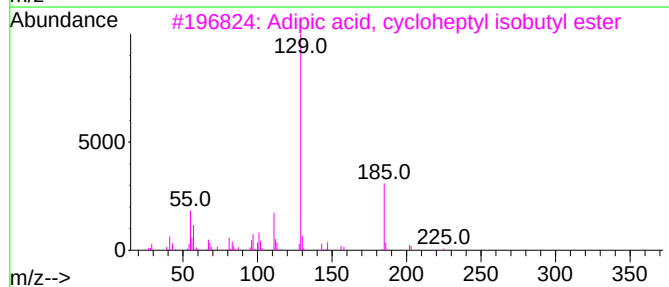
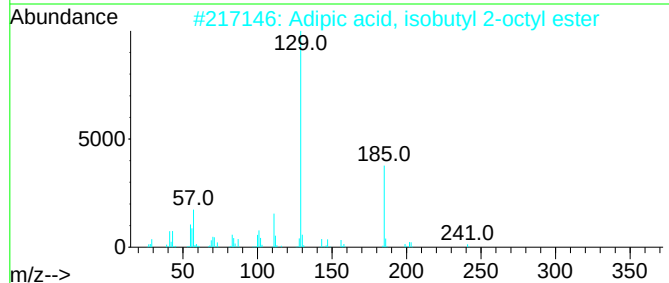
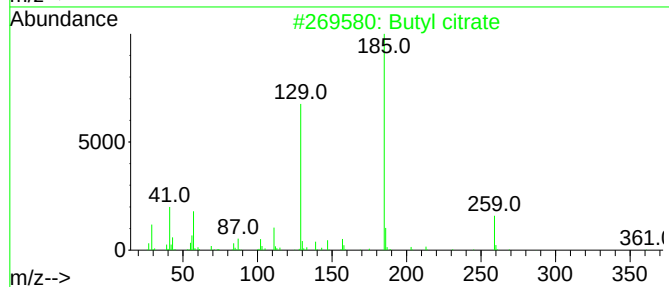
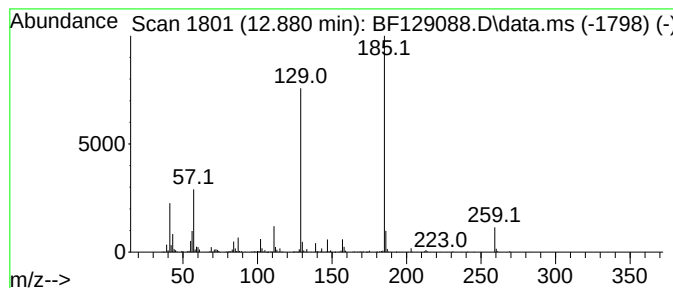
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 Butyl citrate Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.880	2.14 ng	320193	Chrysene-d12	14.139

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butyl citrate	360	C18H32O7	000077-94-1	91
2			Adipic acid, isobutyl 2-octyl ester	314	C18H34O4	1000324-44-5	64
3			Adipic acid, cycloheptyl isobuty...	298	C17H30O4	1000324-71-5	64
4			Adipic acid, butyl 2-methylpent-...	286	C16H30O4	1010353-55-8	56
5			Adipic acid, isobutyl pent-4-en-...	270	C15H26O4	1000354-11-8	56



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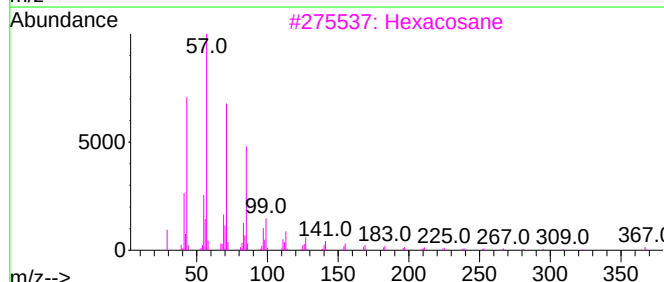
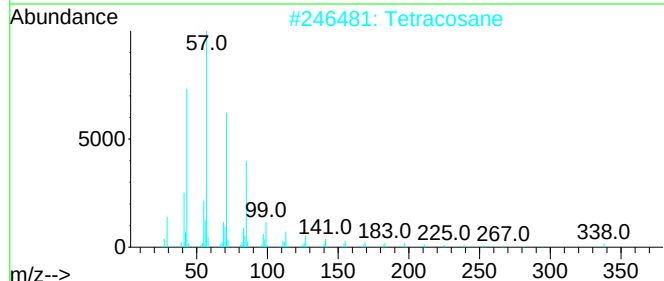
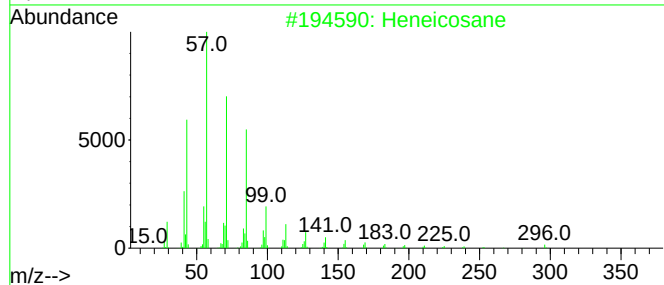
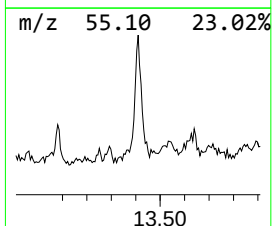
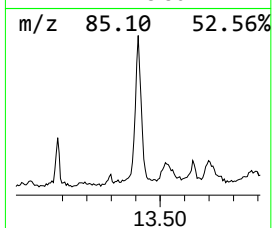
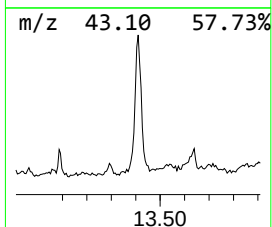
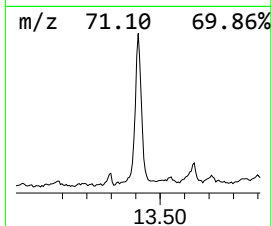
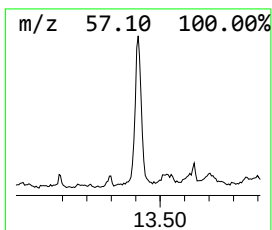
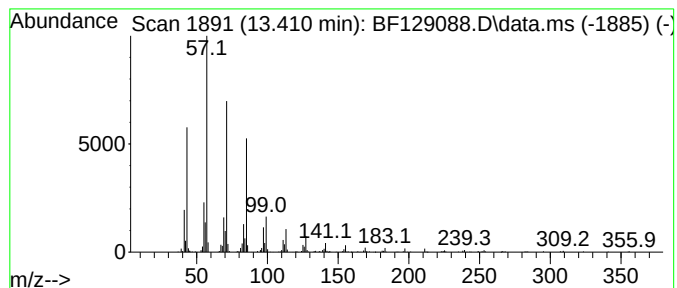
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Heneicosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.410	3.98 ng	594747	Chrysene-d12	14.139

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heneicosane	296	C21H44	000629-94-7	91
2			Tetracosane	338	C24H50	000646-31-1	91
3			Hexacosane	366	C26H54	000630-01-3	91
4			Nonadecane	268	C19H40	000629-92-5	91
5			Eicosane	282	C20H42	000112-95-8	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF070122\
Data File : BF129088.D
Acq On : 01 Jul 2022 12:56
Operator : CG\JU
Sample : N3543-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
KENS-062822-SB18-GW

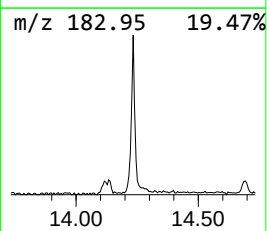
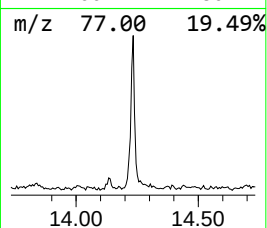
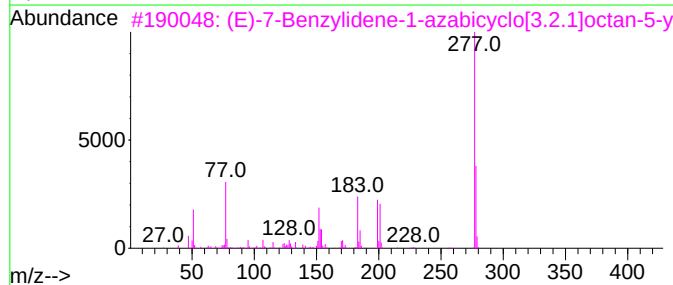
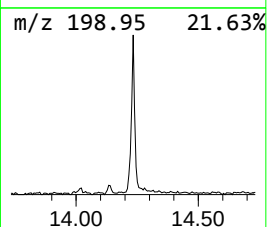
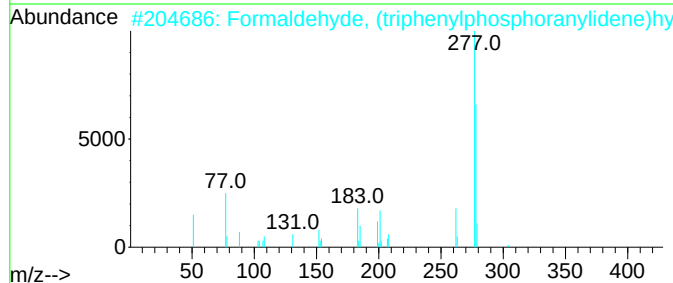
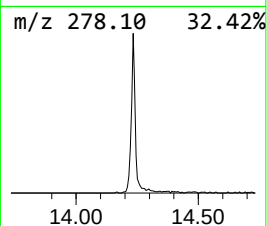
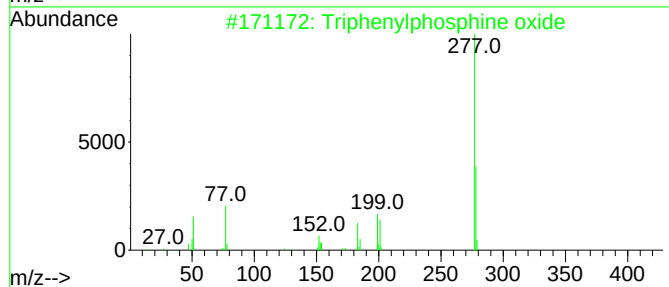
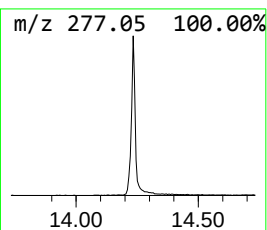
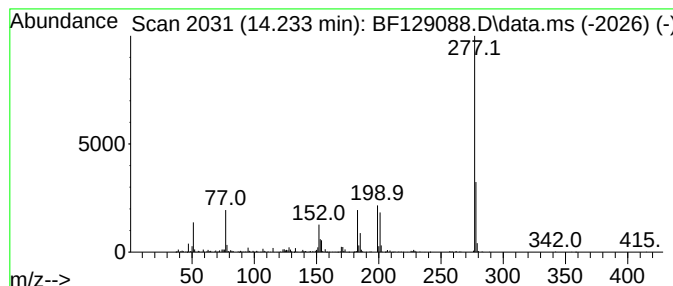
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Triphenylphosphine oxide Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.233	2.52 ng	377126	Chrysene-d12	14.139

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Triphenylphosphine oxide	278	C18H15OP	000791-28-6	95
2			Formaldehyde, (triphenylphosphor...	304	C19H17N2P	015990-54-2	64
3			(E)-7-Benzylidene-1-azabicyclo[3...	293	C15H19N03S	1000483-83-4	64
4			Cobalt, (.eta.<5>-2,4-cyclopentad...	277	C16H15BCo	036682-12-9	32
5			5-Methyl-8-phenylfuro[3',2':5,6]...	277	C16H11N3O2	1000460-07-9	28



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF070122\
Data File : BF129088.D
Acq On : 01 Jul 2022 12:56
Operator : CG\JU
Sample : N3543-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
KENS-062822-SB18-GW

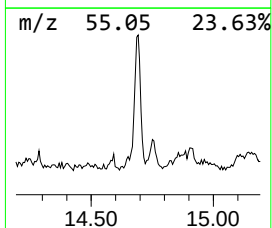
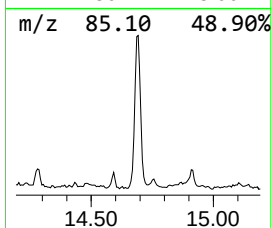
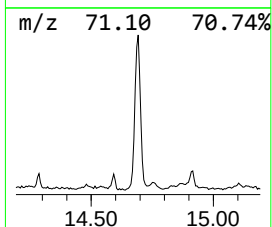
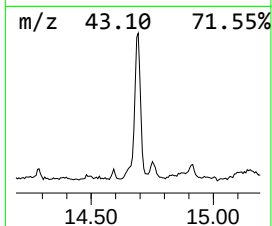
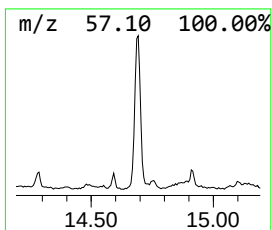
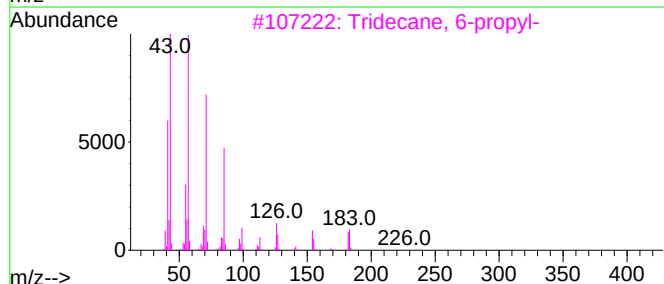
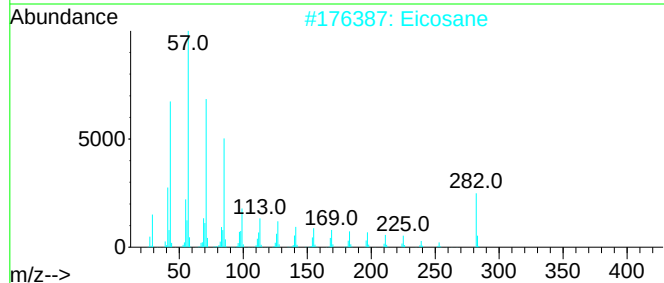
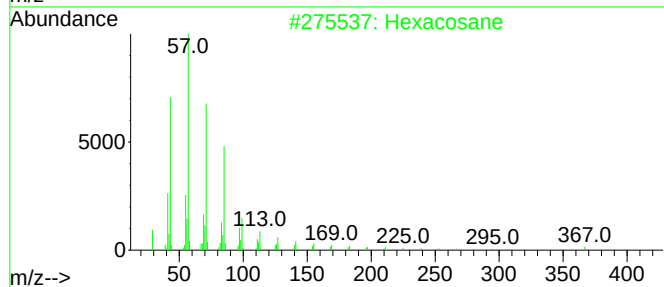
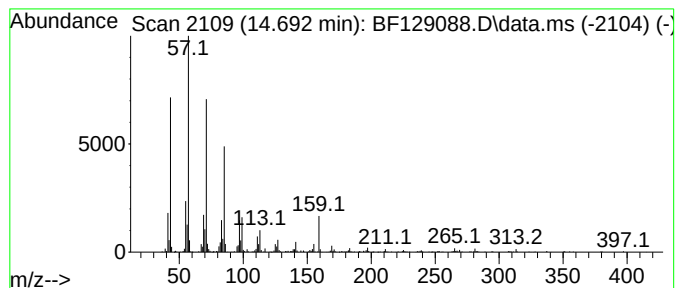
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Hexacosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.692	4.74 ng	709171	Chrysene-d12	14.139

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexacosane	366	C26H54	000630-01-3	93
2			Eicosane	282	C20H42	000112-95-8	90
3			Tridecane, 6-propyl-	226	C16H34	055045-10-8	90
4			Heptacosane	380	C27H56	000593-49-7	90
5			Tetracosane	338	C24H50	000646-31-1	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF070122\
Data File : BF129088.D
Acq On : 01 Jul 2022 12:56
Operator : CG\JU
Sample : N3543-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
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ClientSampleId :
KENS-062822-SB18-GW

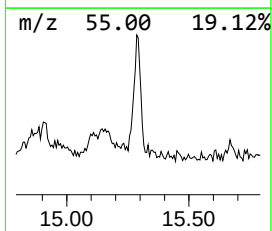
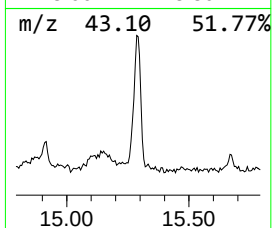
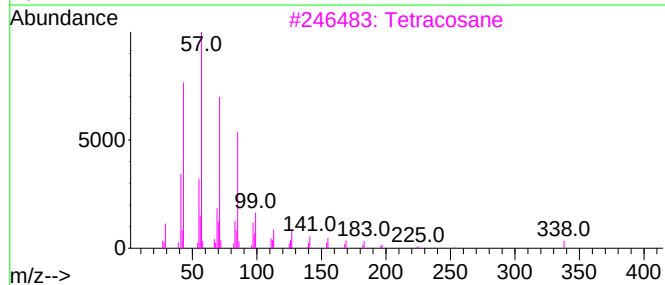
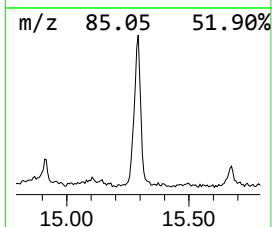
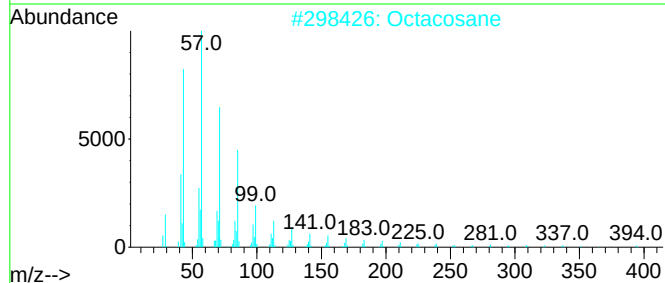
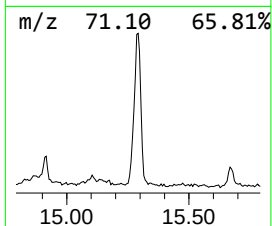
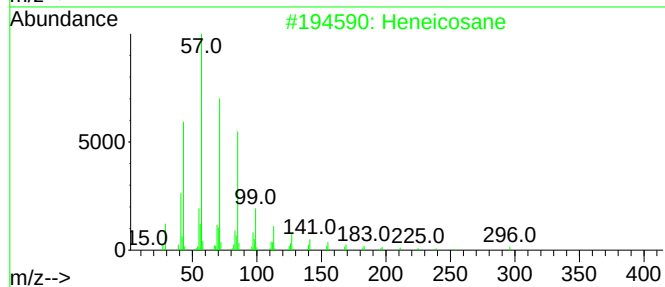
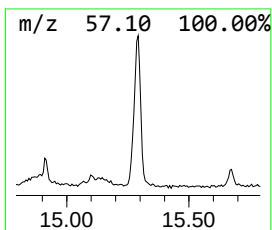
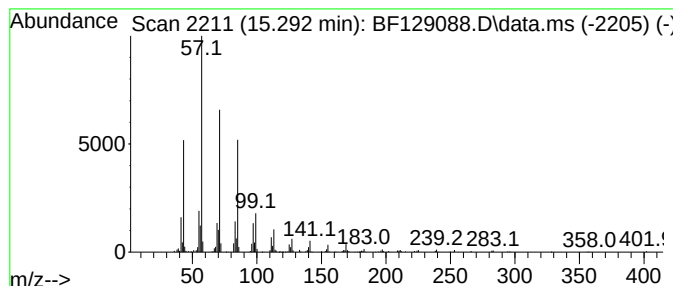
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Octacosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.292	4.97 ng	498884	Perylene-d12	15.663

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Heneicosane	296	C21H44	000629-94-7	91
2		Octacosane	394	C28H58	000630-02-4	91
3		Tetracosane	338	C24H50	000646-31-1	87
4		Octadecane	254	C18H38	000593-45-3	87
5		Pentadecane	212	C15H32	000629-62-9	86



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF070122\
Data File : BF129088.D
Acq On : 01 Jul 2022 12:56
Operator : CG\JU
Sample : N3543-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
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ClientSampleId :
KENS-062822-SB18-GW

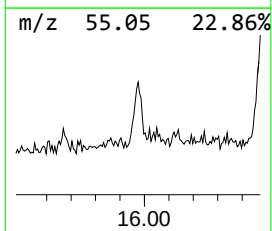
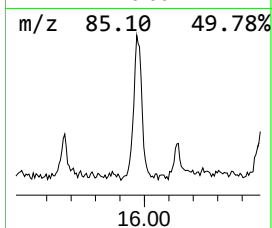
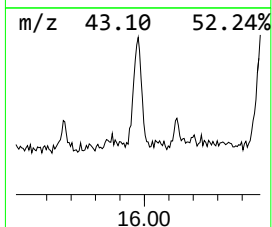
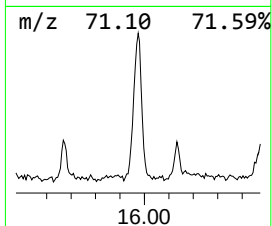
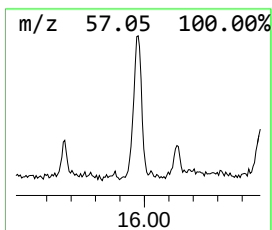
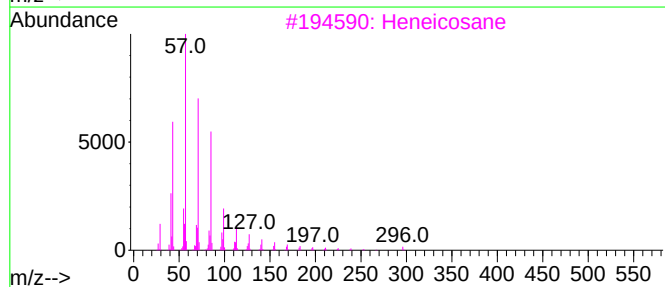
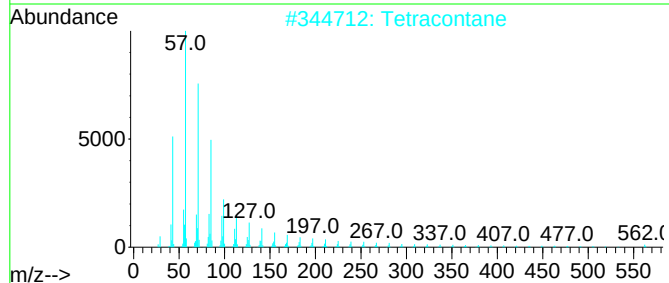
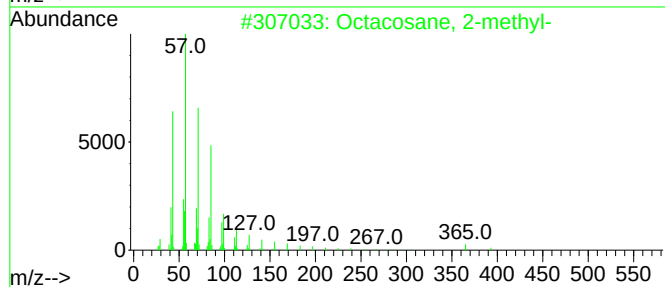
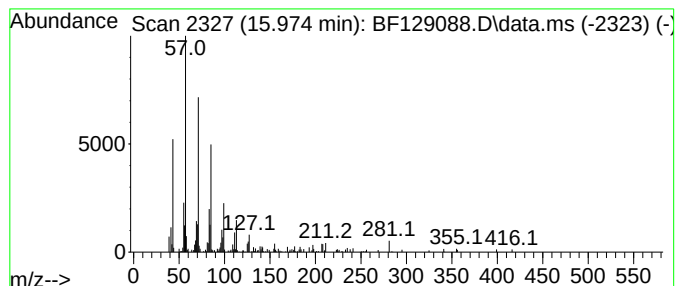
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Octacosane, 2-methyl- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.974	2.14 ng	214537	Perylene-d12	15.663

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Octacosane, 2-methyl-	408	C29H60	001560-98-1	72
2		Tetracontane	563	C40H82	004181-95-7	72
3		Heneicosane	296	C21H44	000629-94-7	72
4		Heneicosane, 11-decyl-	437	C31H64	055320-06-4	72
5		Hentriacontane	437	C31H64	000630-04-6	72



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF070122\
Data File : BF129088.D
Acq On : 01 Jul 2022 12:56
Operator : CG\JU
Sample : N3543-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
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ClientSampleId :
KENS-062822-SB18-GW

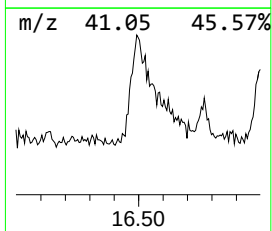
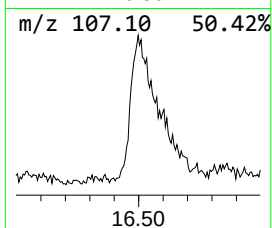
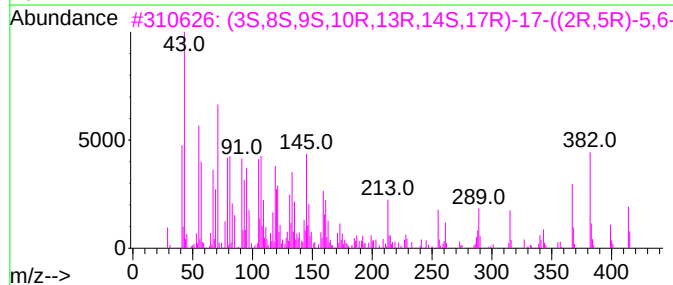
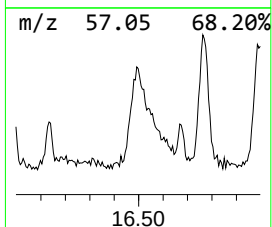
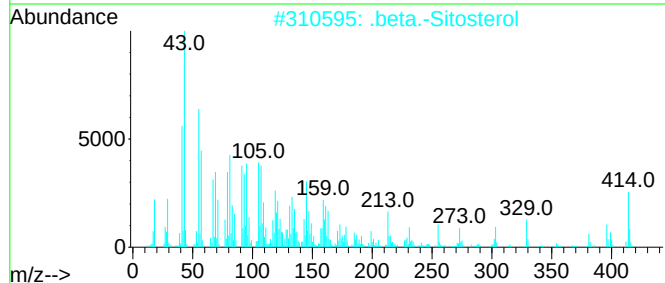
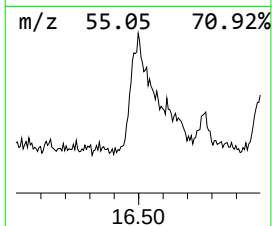
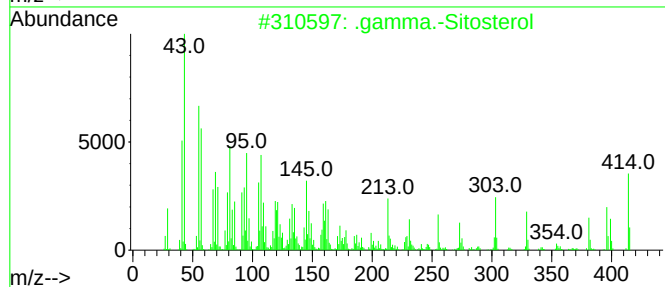
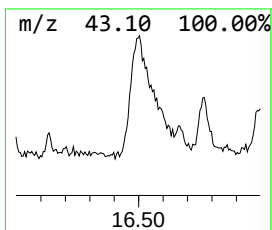
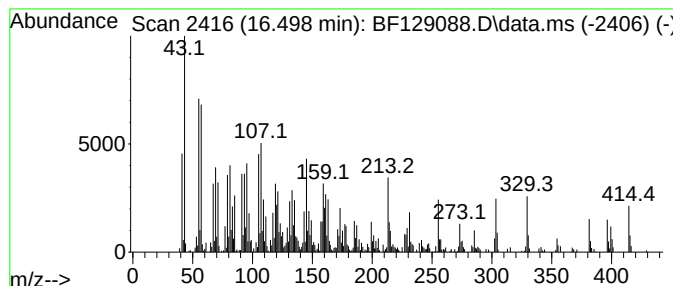
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 .gamma.-Sitosterol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.498	22.04 ng	2213520	Perylene-d12	15.663

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		.gamma.-Sitosterol	414	C29H50O	000083-47-6	99
2		.beta.-Sitosterol	414	C29H50O	000083-46-5	99
3		(3S,8S,9S,10R,13R,14S,17R)-17-((...)	414	C29H50O	029365-29-5	90
4		17-(1,5-Dimethylhexyl)-10,13-dim...	414	C29H50O	1000210-86-9	50
5		Campesterol	400	C28H48O	000474-62-4	49



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF070122\
Data File : BF129088.D
Acq On : 01 Jul 2022 12:56
Operator : CG\JU
Sample : N3543-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
KENS-062822-SB18-GW

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062922.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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Diethyltoluamide	10.375	9.7	ng	1571010	3	9.998	3226770	20.0
n-Hexadecanoic ...	11.998	2.9	ng	471692	4	11.492	3286330	20.0
Octadecanoic acid	12.786	3.5	ng	568045	4	11.492	3286330	20.0
Butyl citrate	12.880	2.1	ng	320193	5	14.139	2990810	20.0
Heneicosane	13.410	4.0	ng	594747	5	14.139	2990810	20.0
Triphenylphosph...	14.233	2.5	ng	377126	5	14.139	2990810	20.0
Hexacosane	14.692	4.7	ng	709171	5	14.139	2990810	20.0
Octacosane	15.292	5.0	ng	498884	6	15.663	2008250	20.0
Octacosane, 2-m...	15.974	2.1	ng	214537	6	15.663	2008250	20.0
.gamma.-Sitosterol	16.498	22.0	ng	2213520	6	15.663	2008250	20.0