

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082421\
 Data File : BF125182.D
 Acq On : 24 Aug 2021 13:28
 Operator : JU/CG
 Sample : M3462-01
 Misc :
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 WP-3

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-BF081821.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF125182.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.193	12	18	23	rVB	1875746	2439419	53.95%	8.081%
2	5.122	510	516	521	rBV	91948	107992	2.39%	0.358%
3	5.528	580	585	588	rBV	1811535	1639547	36.26%	5.431%
4	6.528	751	755	762	rBV	1214900	1029821	22.78%	3.411%
5	6.916	817	821	824	rBV	923671	791452	17.51%	2.622%
6	7.475	911	916	919	rBV	2438451	2332649	51.59%	7.727%
7	8.110	1020	1024	1030	rBV2	49857	98900	2.19%	0.328%
8	8.198	1035	1039	1042	rBV	1297128	1056330	23.36%	3.499%
9	9.269	1217	1221	1225	rBV	4446422	4101164	90.71%	13.585%
10	9.951	1333	1337	1340	rVB	1574299	1213208	26.83%	4.019%
11	10.139	1364	1369	1374	rBV3	42099	52099	1.15%	0.173%
12	10.739	1467	1471	1474	rBV	3080420	2864450	63.36%	9.489%
13	11.145	1536	1540	1544	rBV	89646	78153	1.73%	0.259%
14	11.439	1586	1590	1593	rBV	1507862	1273847	28.17%	4.220%
15	11.957	1671	1678	1693	rBV	1136483	1425530	31.53%	4.722%
16	12.651	1792	1796	1797	rBV2	46370	54533	1.21%	0.181%
17	12.745	1807	1812	1817	rBV	827151	842946	18.64%	2.792%
18	13.027	1855	1860	1863	rBV	4954713	4521225	100.00%	14.977%
19	13.845	1989	1999	2008	rBV2	196336	525351	11.62%	1.740%
20	13.945	2013	2016	2029	rVB5	161317	433814	9.60%	1.437%
21	14.080	2035	2039	2042	rBV	1119717	1014590	22.44%	3.361%
22	14.233	2063	2065	2074	rVB2	36829	53339	1.18%	0.177%
23	14.545	2114	2118	2125	rBV	219897	362857	8.03%	1.202%
24	14.933	2182	2184	2194	rVB3	36878	50253	1.11%	0.166%
25	15.210	2226	2231	2240	rVB2	151775	320467	7.09%	1.062%
26	15.574	2288	2293	2303	rVB	816152	1088298	24.07%	3.605%
27	16.004	2359	2366	2371	rBV2	91832	207657	4.59%	0.688%
28	16.409	2429	2435	2444	rVB2	87753	208140	4.60%	0.689%

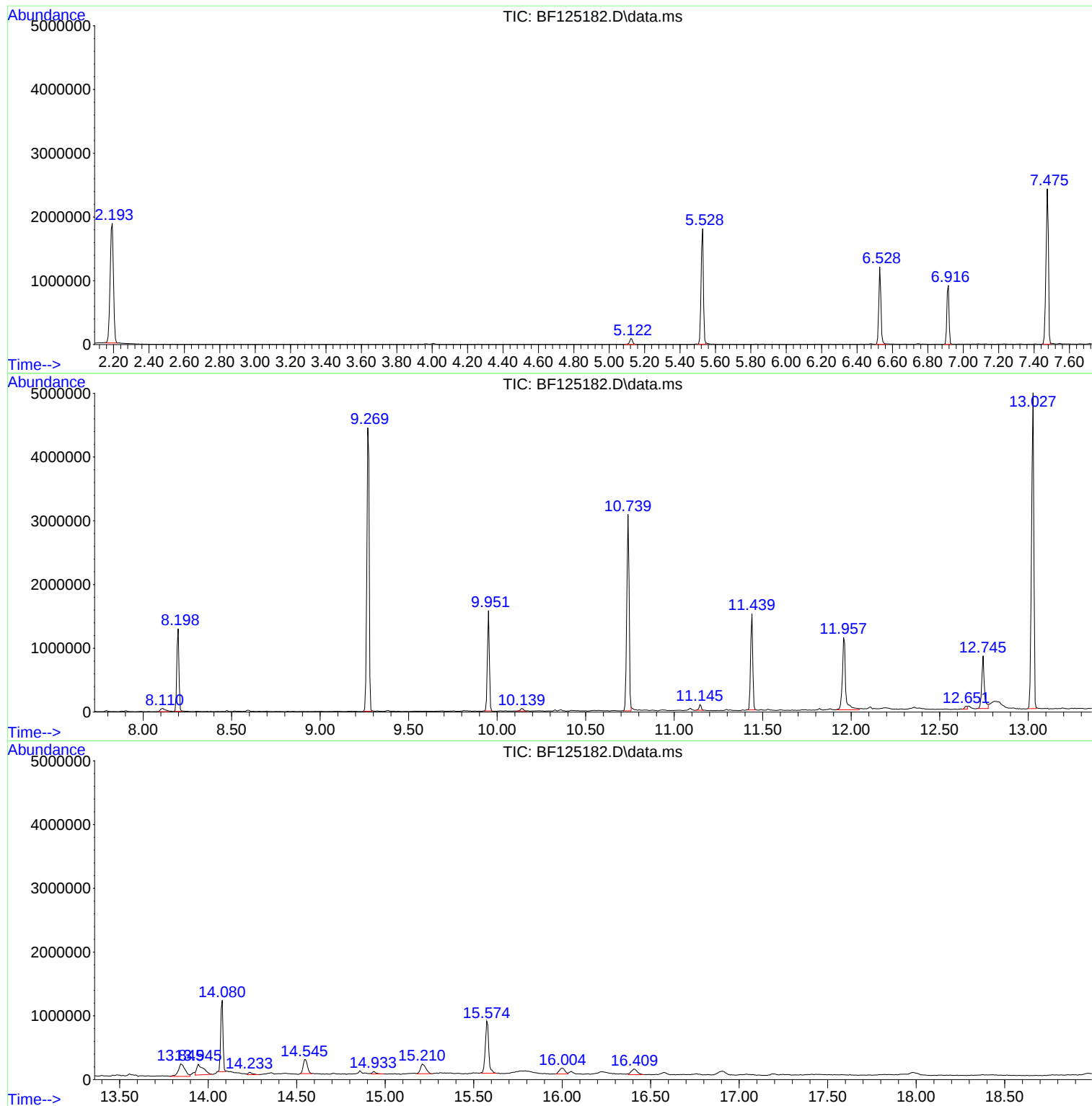
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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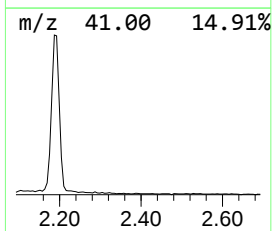
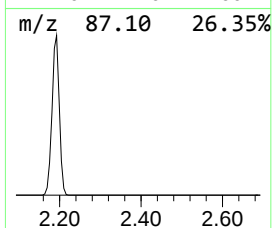
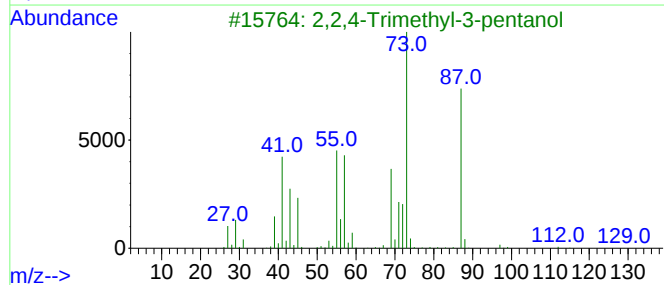
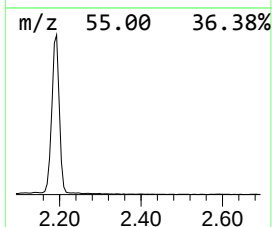
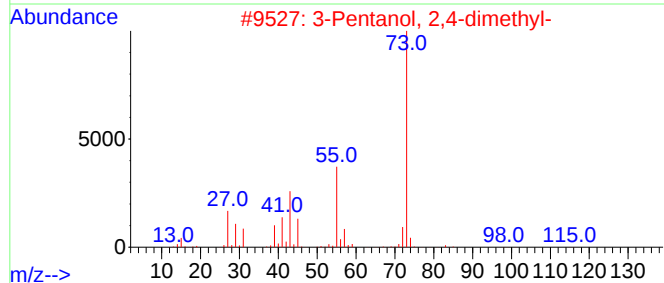
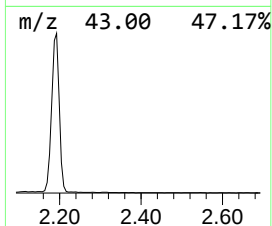
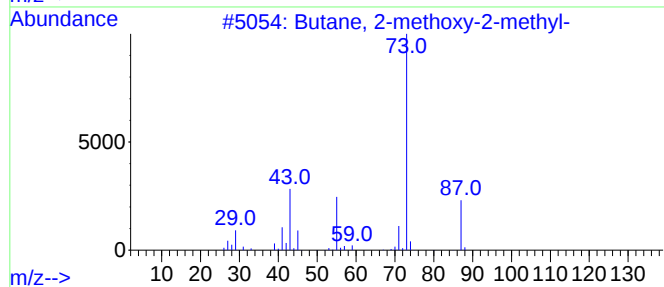
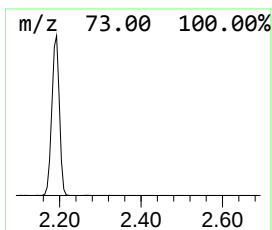
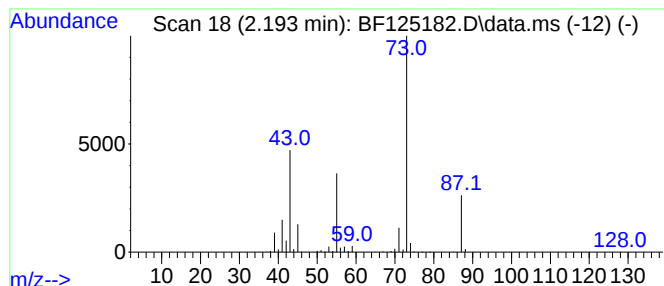
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
2.193	61.64 ng	2439420	1,4-Dichlorobenzene-d4	6.916

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2			3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	43
3			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
4			Silane, tetramethyl-	88	C4H12Si	000075-76-3	38
5			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	23



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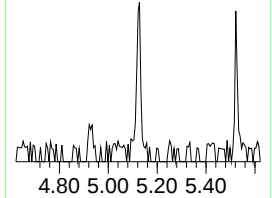
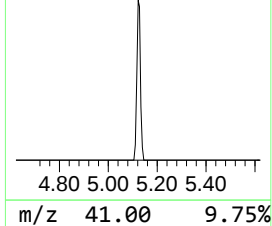
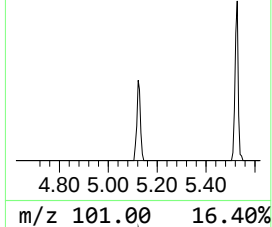
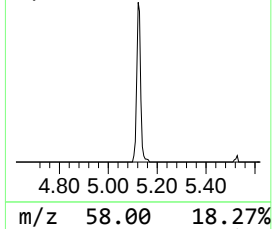
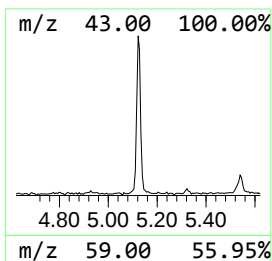
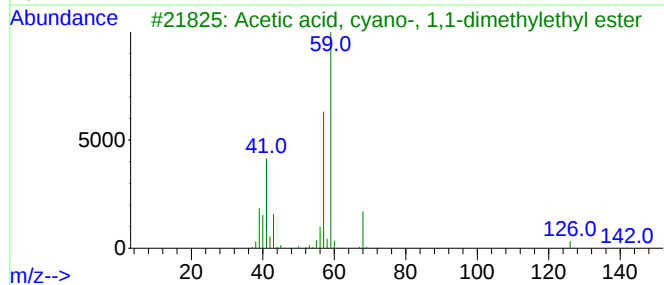
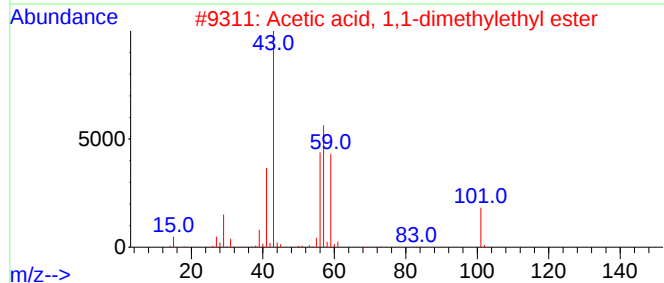
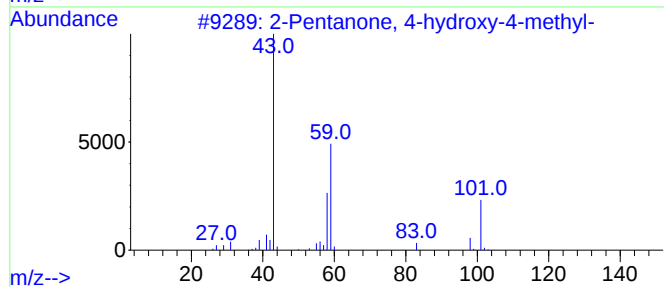
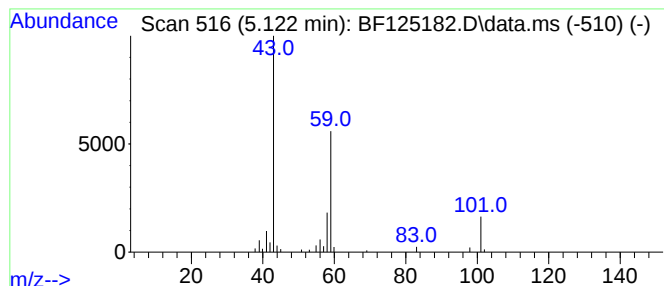
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Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.122	2.73 ng	107992	1,4-Dichlorobenzene-d4	6.916

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	38
3			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	37
4			3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
5			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16



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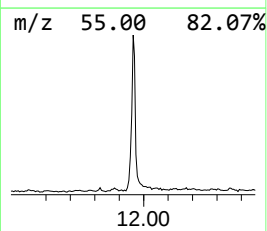
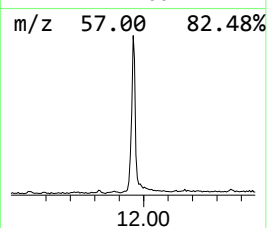
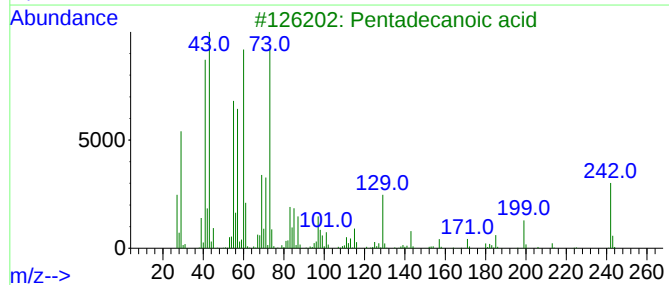
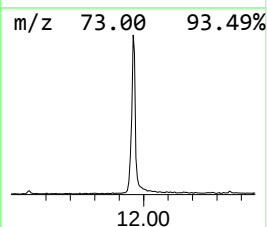
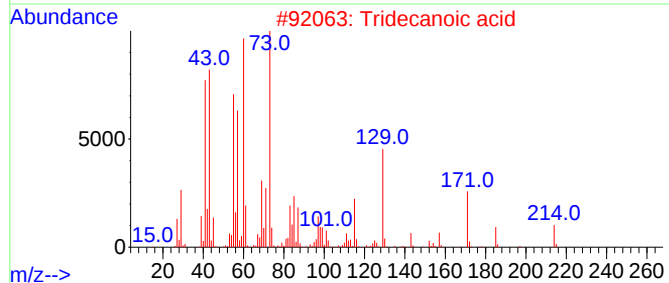
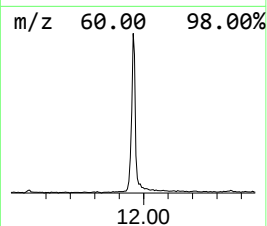
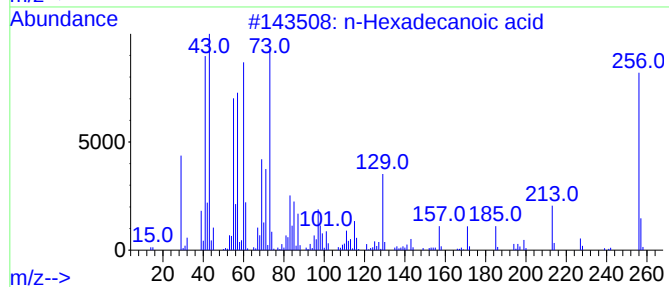
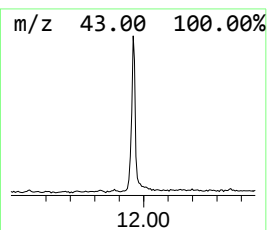
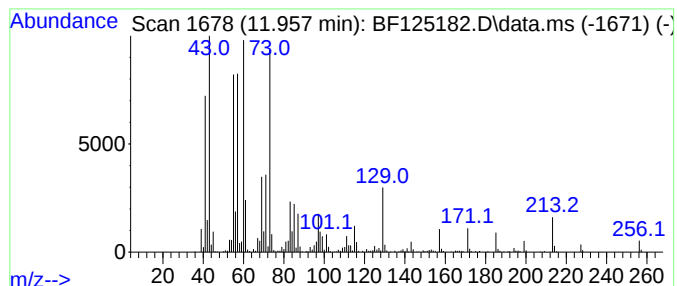
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Peak Number 3 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.957	22.38 ng	1425530	Phenanthrene-d10	11.439

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2			Tridecanoic acid	214	C13H26O2	000638-53-9	93
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	83
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	78
5			Dodecanoic acid	200	C12H24O2	000143-07-7	76



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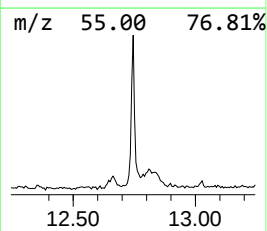
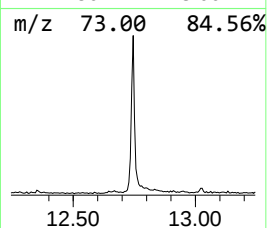
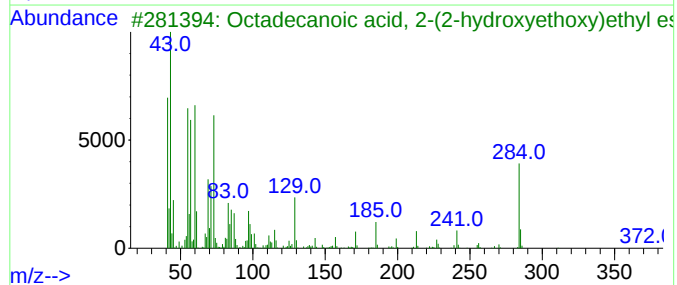
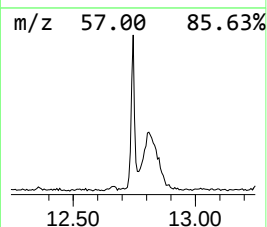
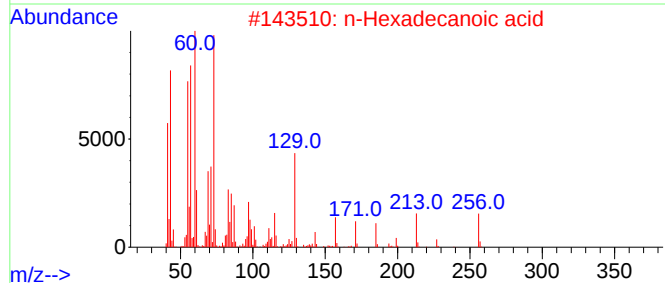
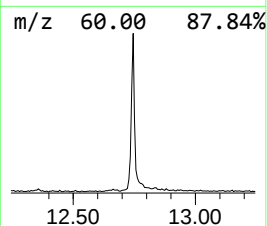
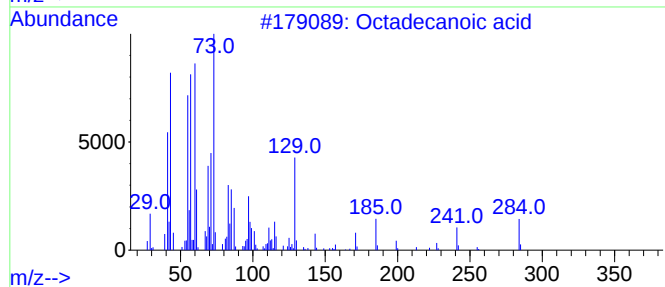
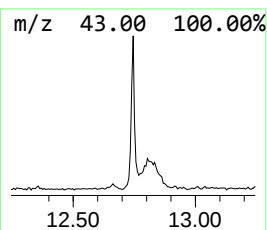
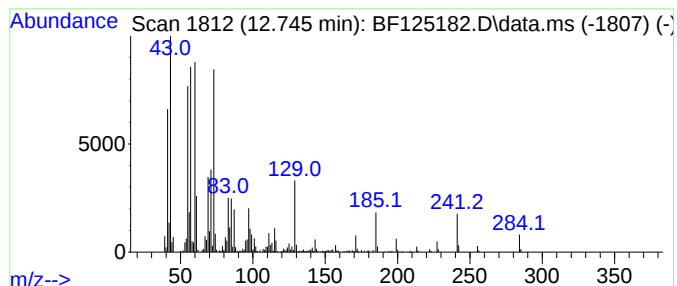
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Peak Number 4 Octadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.745	13.23 ng	842946	Phenanthrene-d10	11.439

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	93
2			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	91
3			Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	87
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	83
5			Undecanoic acid	186	C11H22O2	000112-37-8	83



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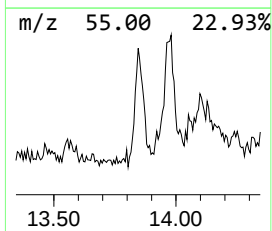
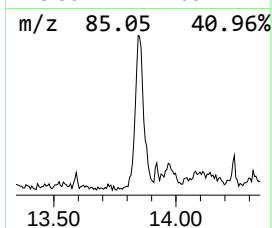
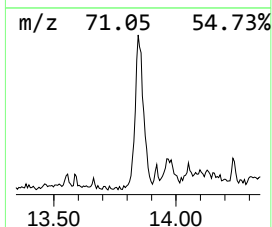
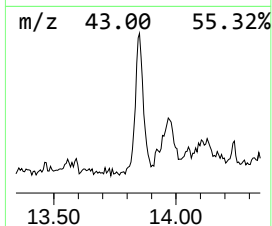
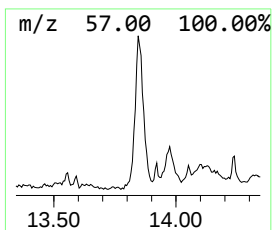
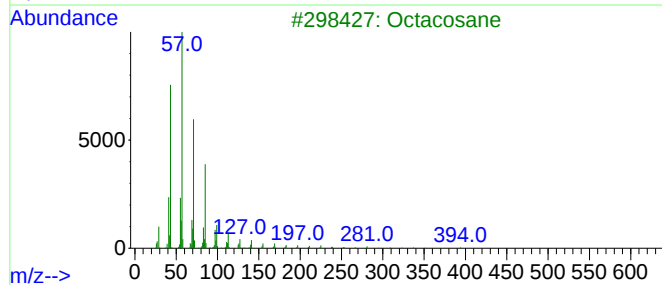
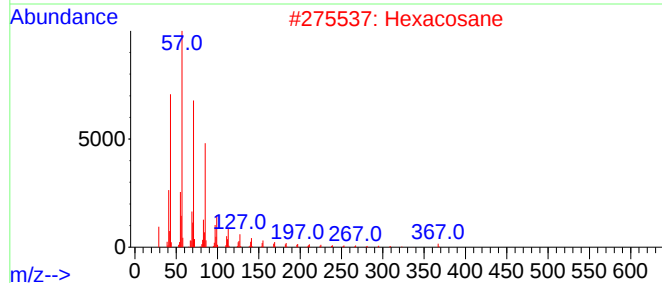
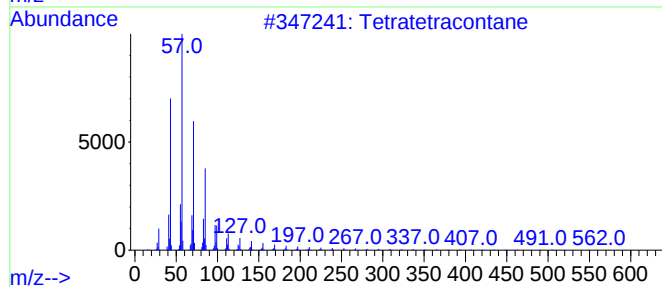
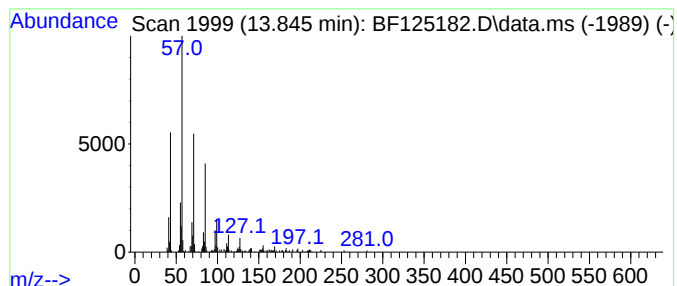
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Peak Number 5 Tetratetracontane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.845	10.36 ng	525351	Chrysene-d12	14.080

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetratetracontane	619	C44H90	007098-22-8	91
2			Hexacosane	366	C26H54	000630-01-3	91
3			Octacosane	394	C28H58	000630-02-4	90
4			Heneicosane	296	C21H44	000629-94-7	90
5			Heptacosane	380	C27H56	000593-49-7	87



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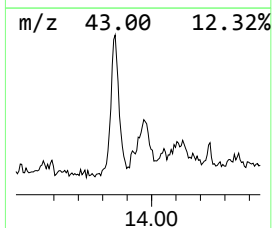
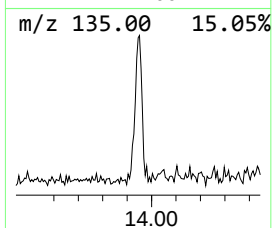
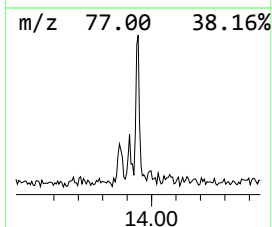
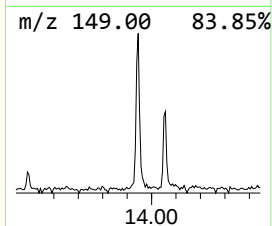
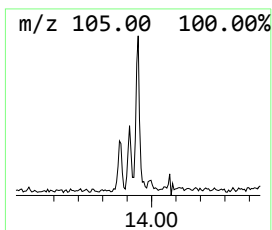
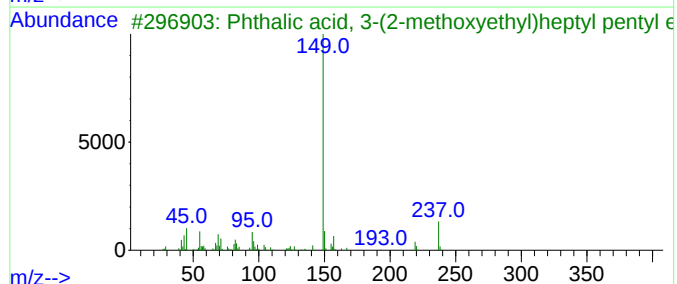
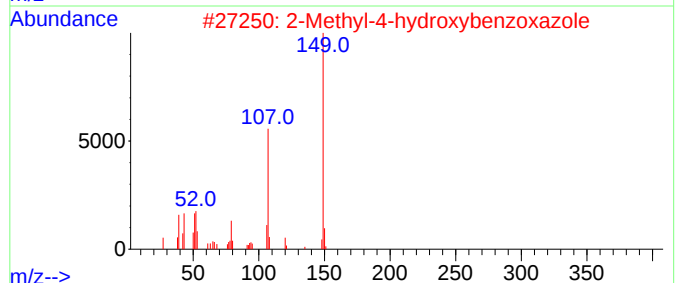
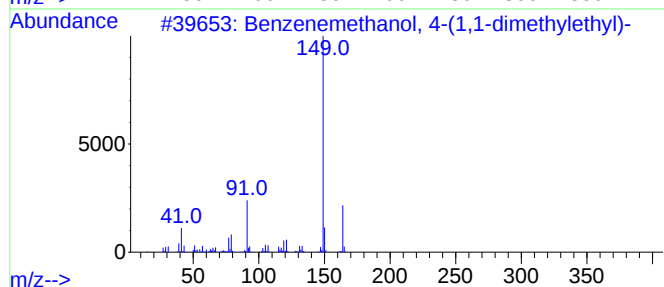
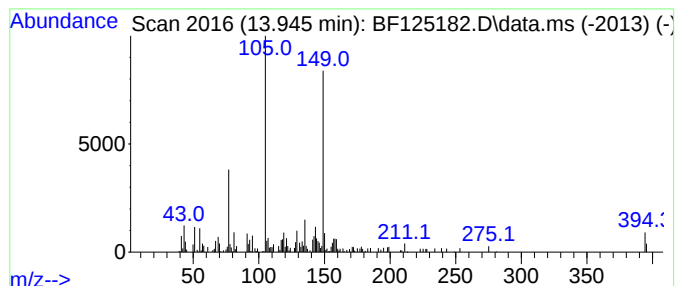
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 unknown13.945 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.945	8.55 ng	433814	Chrysene-d12	14.080

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzenemethanol, 4-(1,1-dimethyl...	164	C11H16O	000877-65-6	38
2			2-Methyl-4-hydroxybenzoxazole	149	C8H7NO2	051110-60-2	30
3			Phthalic acid, 3-(2-methoxyethyl...	392	C23H36O5	1000315-39-5	27
4			Phthalic acid, 2-chloroethyl dec...	368	C20H29ClO4	1000315-77-5	27
5			Phthalic acid, but-3-yn-2-yl cyc...	314	C19H22O4	1000315-75-8	27



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082421\
Data File : BF125182.D
Acq On : 24 Aug 2021 13:28
Operator : JU/CG
Sample : M3462-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WP-3

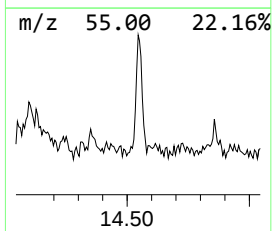
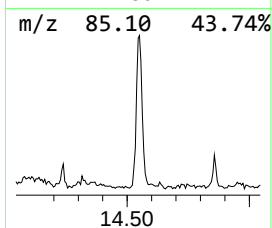
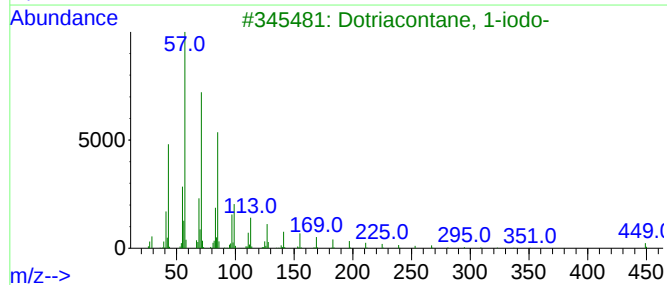
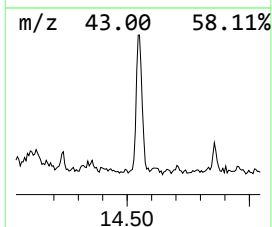
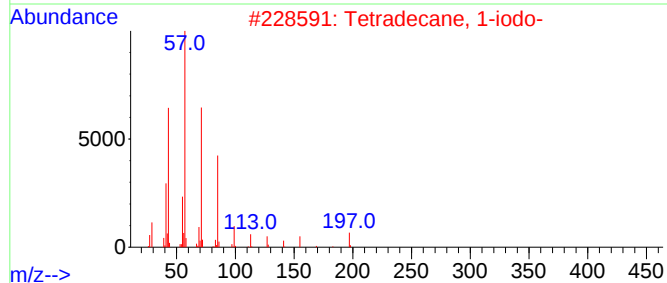
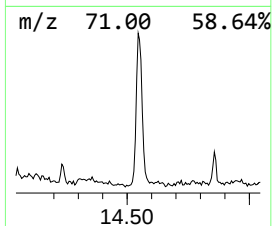
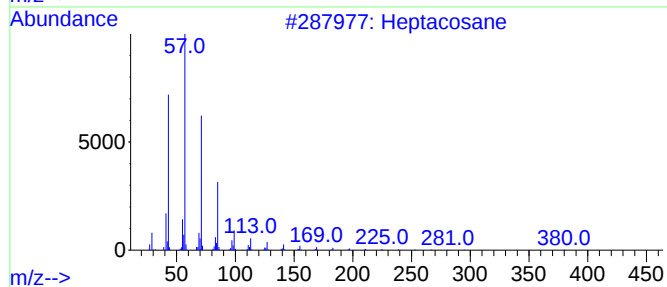
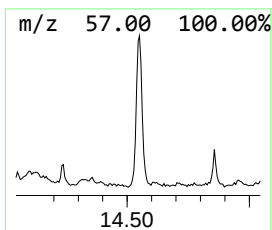
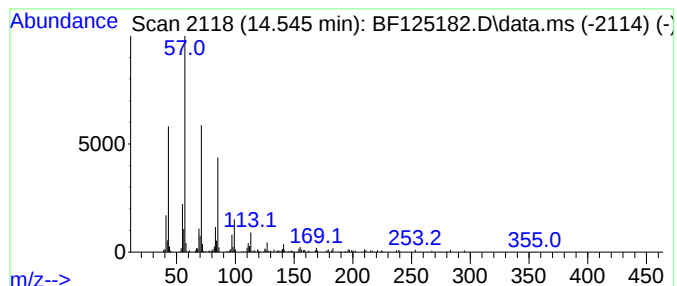
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Heptacosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.545	7.15 ng	362857	Chrysene-d12	14.080

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptacosane	380	C27H56	000593-49-7	91
2			Tetradecane, 1-iodo-	324	C14H29I	019218-94-1	91
3			Dotriacontane, 1-iodo-	576	C32H65I	1000406-32-4	91
4			Eicosane	282	C20H42	000112-95-8	91
5			Hexacosane	366	C26H54	000630-01-3	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082421\
Data File : BF125182.D
Acq On : 24 Aug 2021 13:28
Operator : JU/CG
Sample : M3462-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WP-3

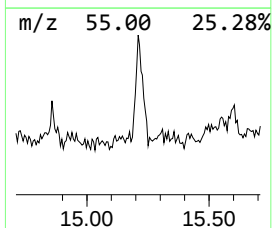
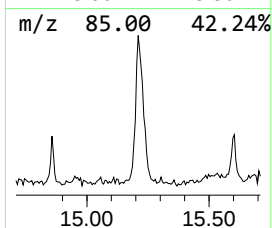
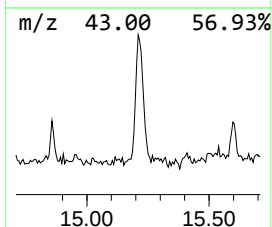
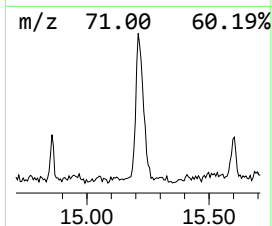
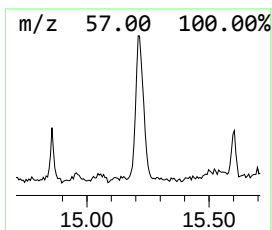
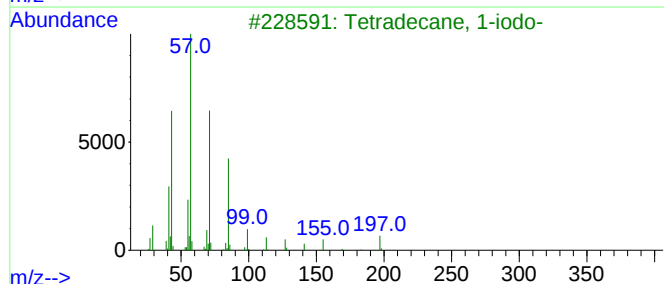
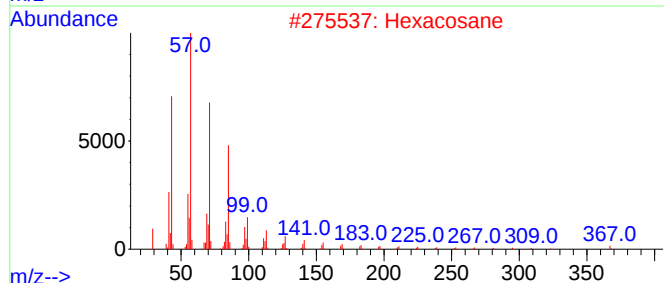
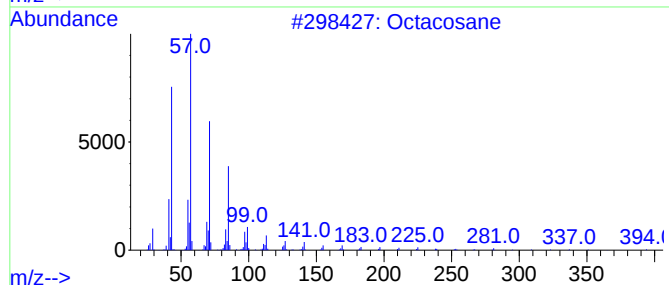
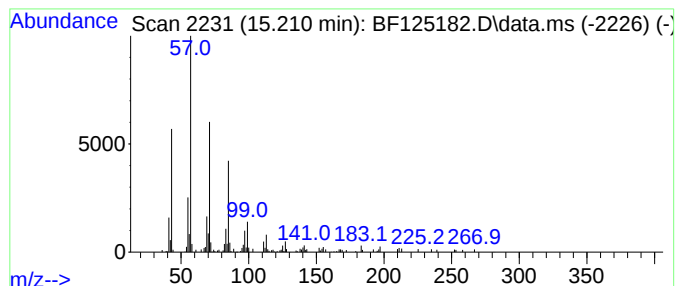
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Octacosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.210	5.89 ng	320467	Perylene-d12	15.574

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octacosane	394	C28H58	000630-02-4	87
2			Hexacosane	366	C26H54	000630-01-3	86
3			Tetradecane, 1-iodo-	324	C14H29I	019218-94-1	80
4			Heptacosane	380	C27H56	000593-49-7	80
5			Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	80



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082421\
Data File : BF125182.D
Acq On : 24 Aug 2021 13:28
Operator : JU/CG
Sample : M3462-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WP-3

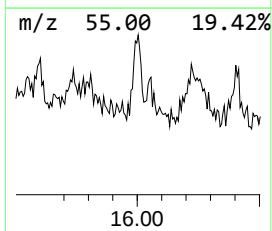
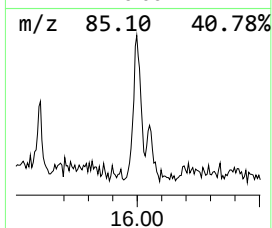
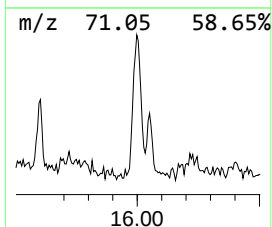
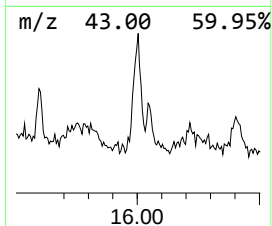
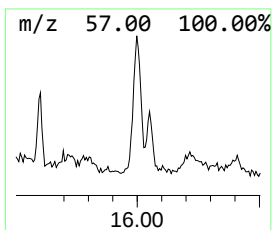
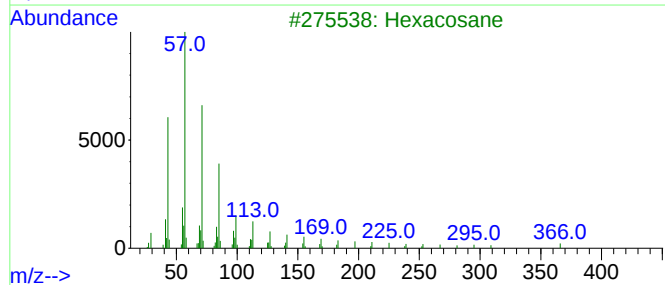
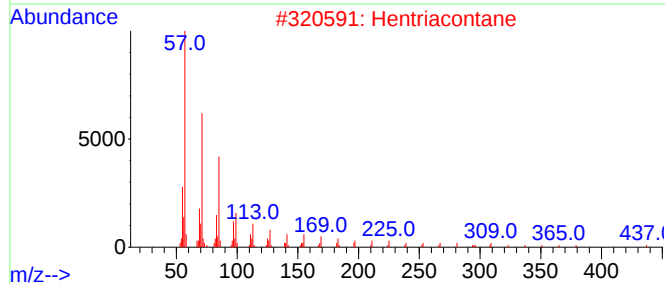
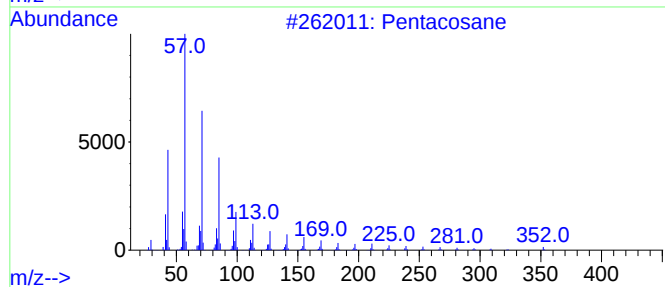
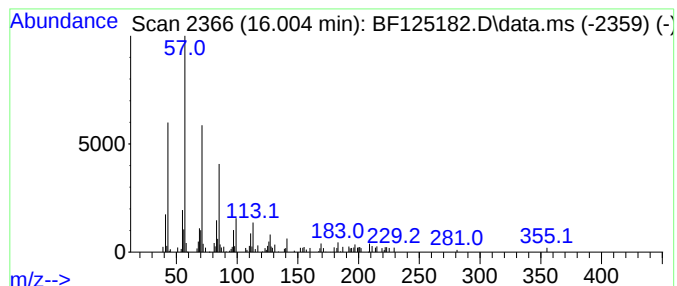
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Pentacosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.004	3.82 ng	207657	Perylene-d12	15.574

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentacosane	352	C25H52	000629-99-2	91
2			Hentriacontane	437	C31H64	000630-04-6	91
3			Hexacosane	366	C26H54	000630-01-3	90
4			Octacosane	394	C28H58	000630-02-4	90
5			Docosane, 11-decyl-	451	C32H66	055401-55-3	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082421\
Data File : BF125182.D
Acq On : 24 Aug 2021 13:28
Operator : JU/CG
Sample : M3462-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WP-3

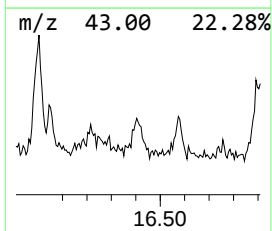
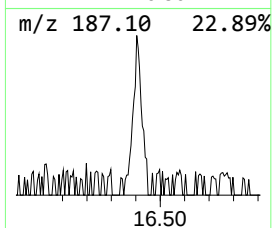
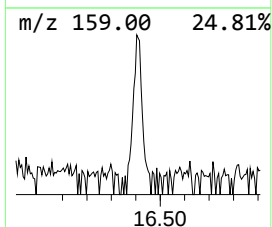
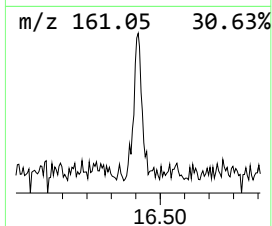
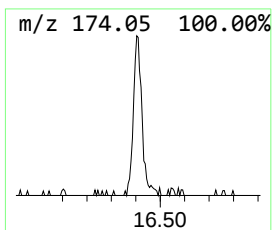
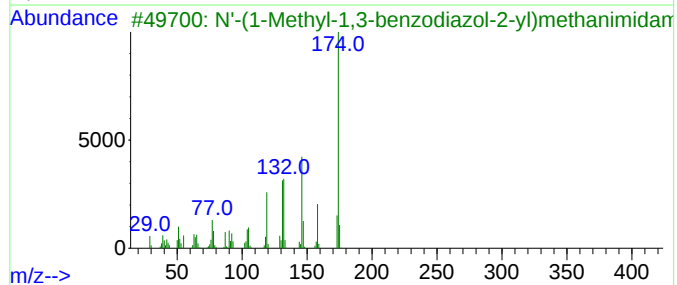
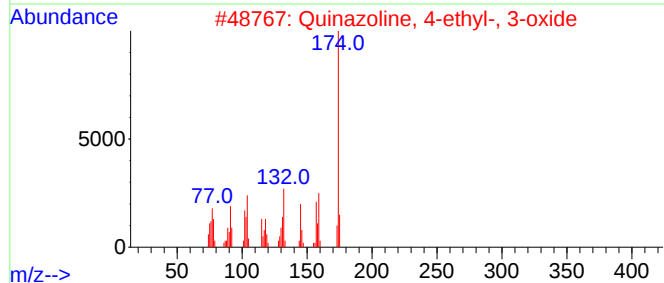
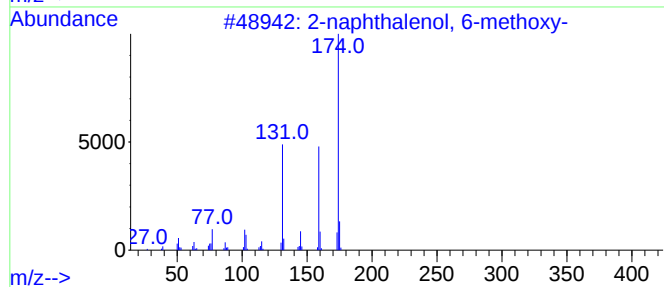
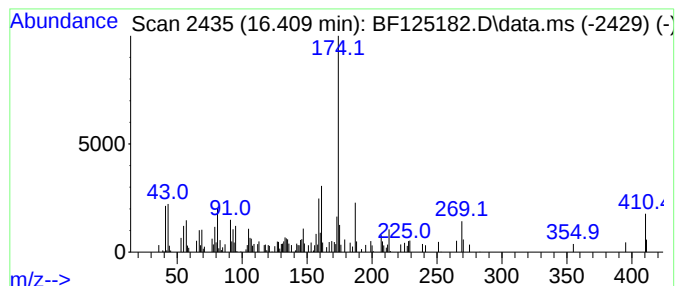
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 unknown16.410 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.410	3.83 ng	208140	Perylene-d12	15.574

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-naphthalenol, 6-methoxy-	174	C11H10O2	1000404-68-0	43
2			Quinazoline, 4-ethyl-, 3-oxide	174	C10H10N2O	037920-74-4	43
3			N'-(1-Methyl-1,3-benzodiazol-2-yl)...	174	C9H10N4	1000443-47-8	38
4			4-(3-Fluorophenyl)pyrimidine	174	C10H7FN2	068049-18-3	38
5			N-Benzyl-2-cyano-acetamide	174	C10H10N2O	1000300-42-1	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082421\
Data File : BF125182.D
Acq On : 24 Aug 2021 13:28
Operator : JU/CG
Sample : M3462-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WP-3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.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-...	5.122	2.7	ng	107992	1	6.916	791452	20.0
n-Hexadecanoic ...	11.957	22.4	ng	1425530	4	11.439	1273850	20.0
Octadecanoic acid	12.745	13.2	ng	842946	4	11.439	1273850	20.0
Tetratetracontane	13.845	10.4	ng	525351	5	14.080	1014590	20.0
unknown13.945	13.945	8.6	ng	433814	5	14.080	1014590	20.0
Heptacosane	14.545	7.2	ng	362857	5	14.080	1014590	20.0
Octacosane	15.210	5.9	ng	320467	6	15.574	1088300	20.0
Pentacosane	16.004	3.8	ng	207657	6	15.574	1088300	20.0
unknown16.410	16.410	3.8	ng	208140	6	15.574	1088300	20.0