

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102920\
 Data File : BF122171.D
 Acq On : 29 Oct 2020 18:45
 Operator : JU/CG
 Sample : L4552-04
 Misc :
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 VW-STONE-B

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-BF101220.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF122171.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.340	550	553	579	rBV	2457288	2862785	88.61%	12.145%
2	6.369	724	728	755	rBV	2503426	2953221	91.41%	12.528%
3	6.716	784	787	797	rVB	622299	588014	18.20%	2.494%
4	7.287	880	884	907	rBV	1959309	1905831	58.99%	8.085%
5	7.998	1001	1005	1021	rBV	797716	780446	24.16%	3.311%
6	8.810	1140	1143	1156	rBV	87391	174225	5.39%	0.739%
7	9.069	1183	1187	1199	rBV	3331153	3230748	100.00%	13.706%
8	9.469	1252	1255	1267	rBV	264088	246795	7.64%	1.047%
9	9.745	1299	1302	1310	rBV	1047970	896731	27.76%	3.804%
10	10.539	1433	1437	1448	rBV	2101206	2223834	68.83%	9.434%
11	11.233	1552	1555	1562	rBV	962753	942498	29.17%	3.998%
12	11.775	1643	1647	1652	rBV	562343	587085	18.17%	2.491%
13	12.557	1777	1780	1785	rBV2	160821	185364	5.74%	0.786%
14	12.822	1820	1825	1828	rBV	3195056	2928939	90.66%	12.425%
15	13.727	1976	1979	1997	rVB2	332130	639316	19.79%	2.712%
16	13.880	2002	2005	2018	rVB	668625	706056	21.85%	2.995%
17	14.939	2183	2185	2190	rVB	55597	59931	1.86%	0.254%
18	15.315	2244	2249	2260	rVB	493593	701752	21.72%	2.977%
19	15.486	2275	2278	2284	rVB6	31339	45005	1.39%	0.191%
20	15.698	2310	2314	2319	rVB	45292	64539	2.00%	0.274%
21	15.786	2324	2329	2339	rBV4	56353	175685	5.44%	0.745%
22	16.168	2389	2394	2397	rBV3	25132	55164	1.71%	0.234%
23	16.204	2397	2400	2407	rVB	43590	70289	2.18%	0.298%
24	16.439	2435	2440	2445	rVB2	34679	57771	1.79%	0.245%
25	16.704	2480	2485	2495	rVB3	29099	65750	2.04%	0.279%
26	16.857	2506	2511	2519	rBV9	22798	74048	2.29%	0.314%
27	16.945	2521	2526	2534	rVB2	81533	160683	4.97%	0.682%
28	17.227	2566	2574	2586	rBV2	37266	135556	4.20%	0.575%
29	17.345	2589	2594	2602	rVB6	22600	54511	1.69%	0.231%

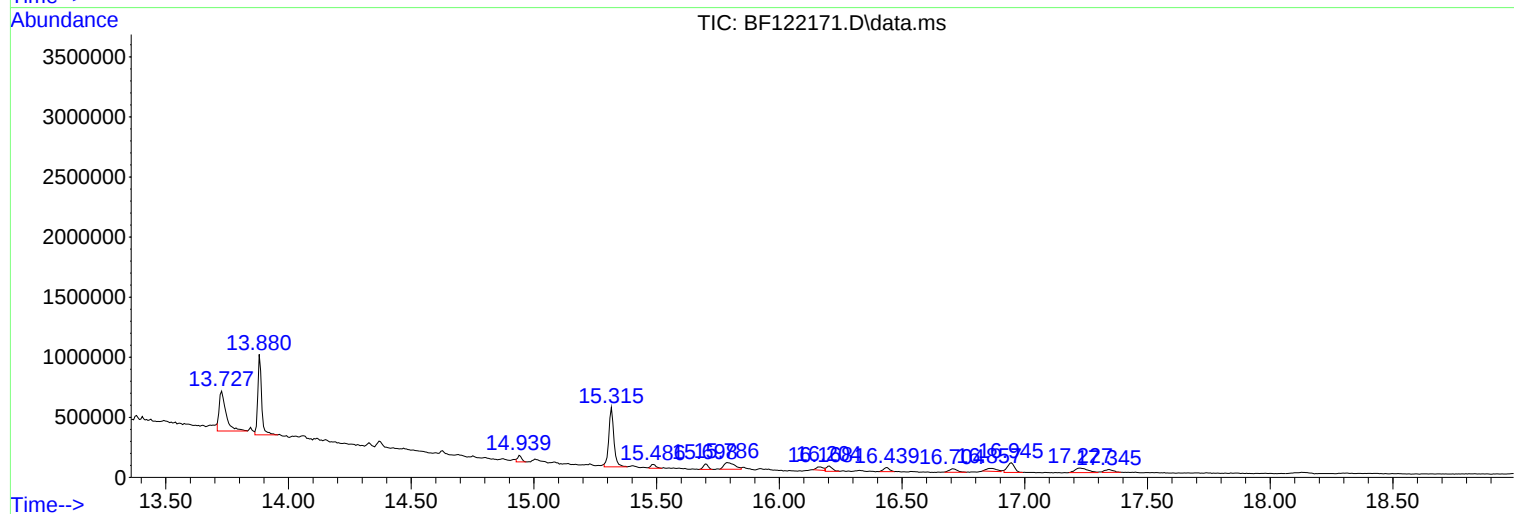
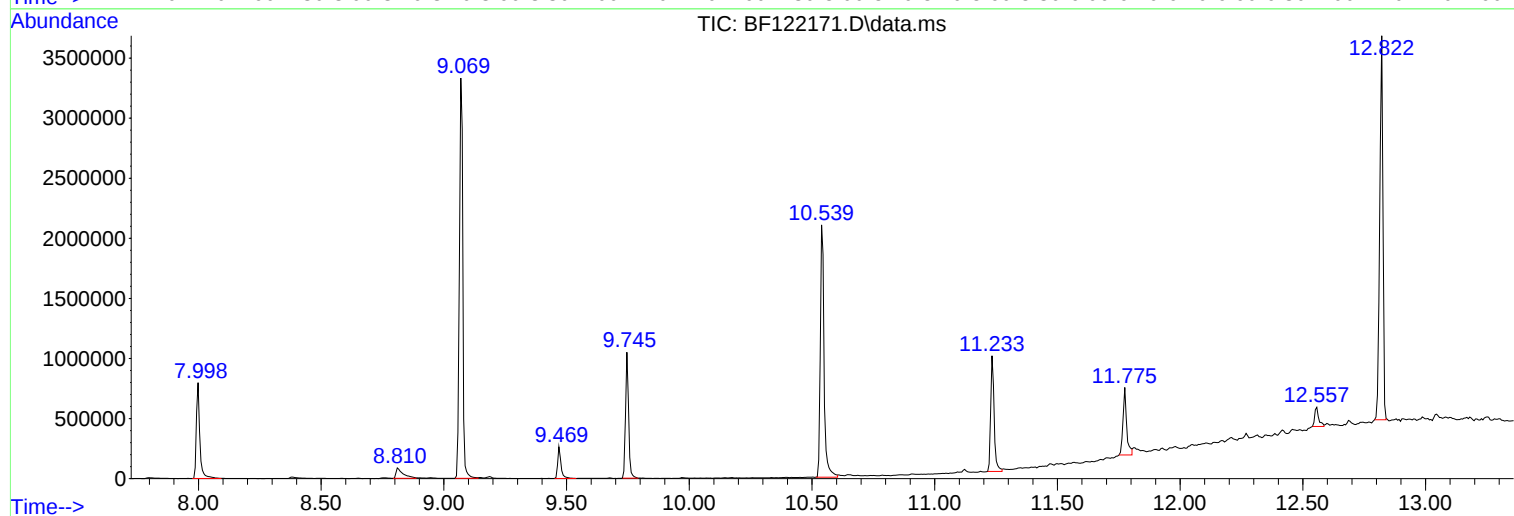
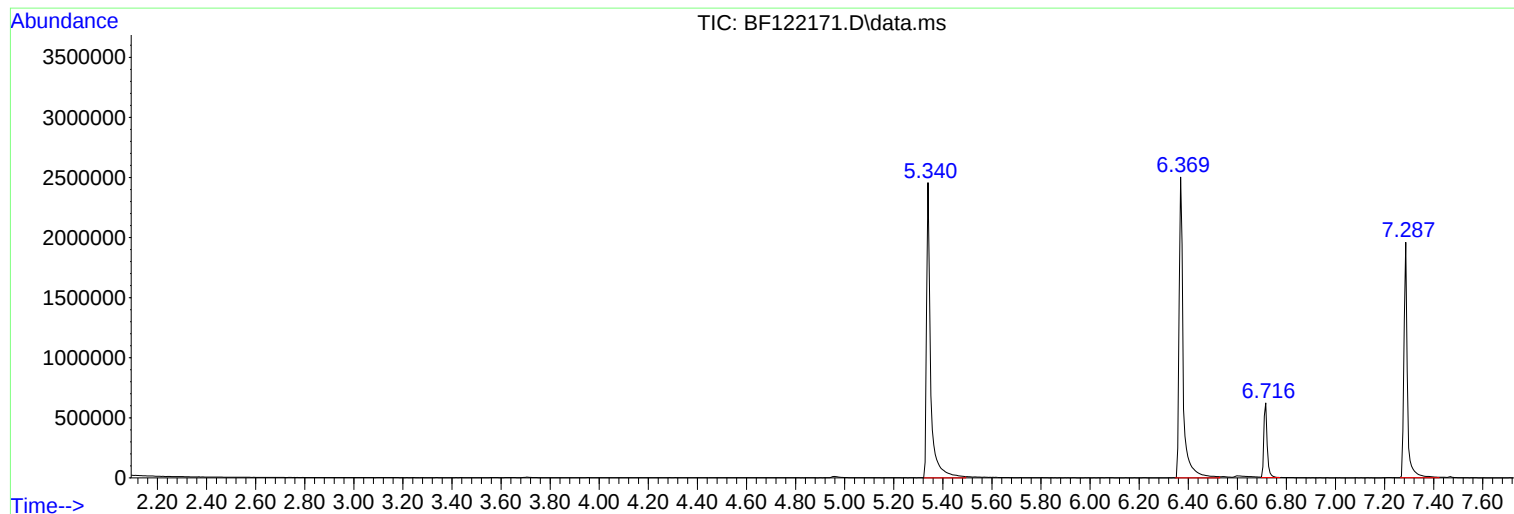
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101220.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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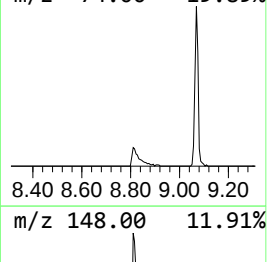
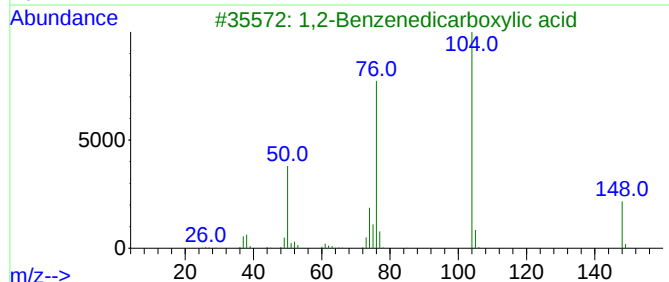
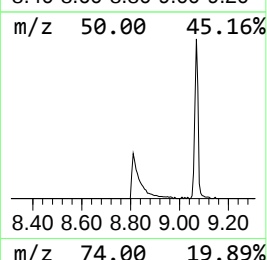
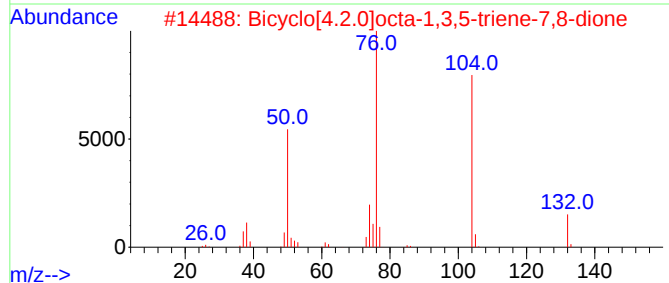
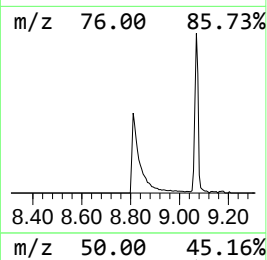
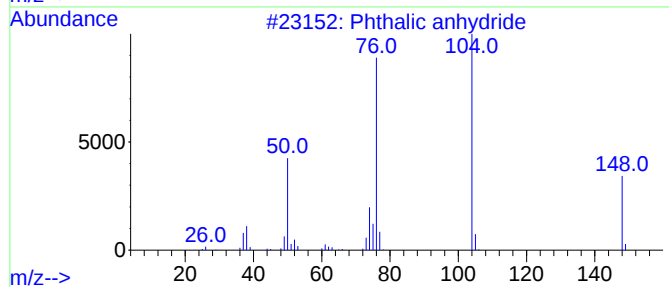
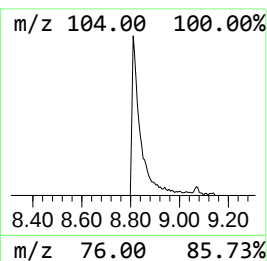
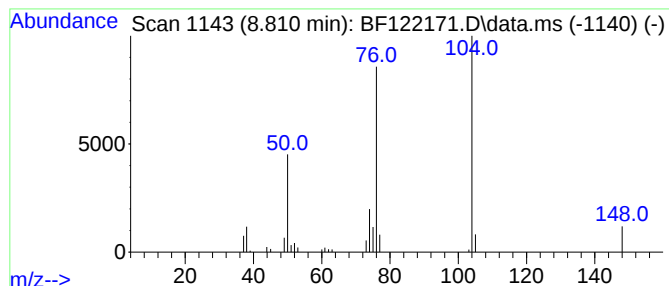
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Phthalic anhydride Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.810	4.46 ng	174225	Naphthalene-d8	7.998

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Phthalic anhydride	148	C8H4O3	000085-44-9	95
2			Bicyclo[4.2.0]octa-1,3,5-triene...	132	C8H4O2	006383-11-5	86
3			1,2-Benzenedicarboxylic acid	166	C8H6O4	000088-99-3	83
4			N-[2-Acetamidoethylthio]phthalimide	264	C12H12N2O3S	025158-14-9	64
5			Phthalimide	147	C8H5NO2	000085-41-6	56



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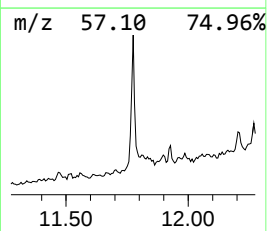
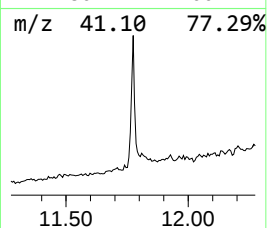
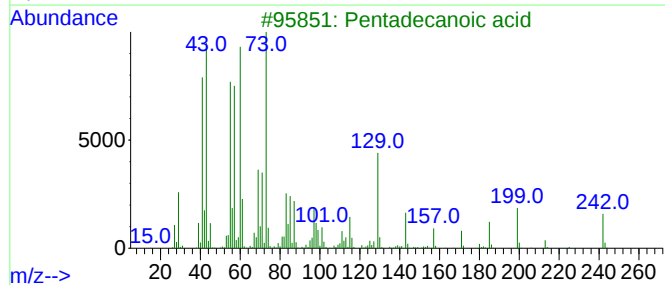
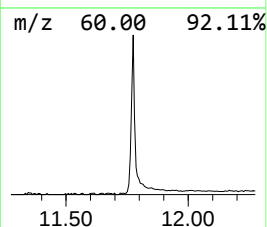
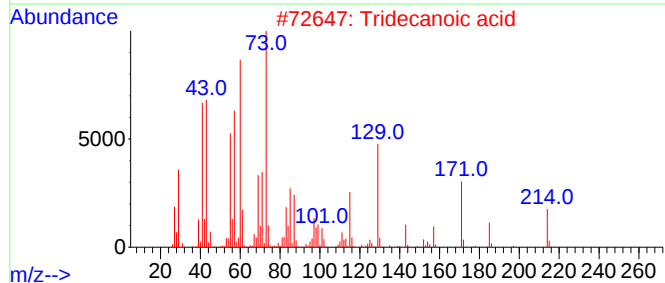
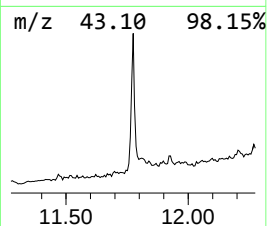
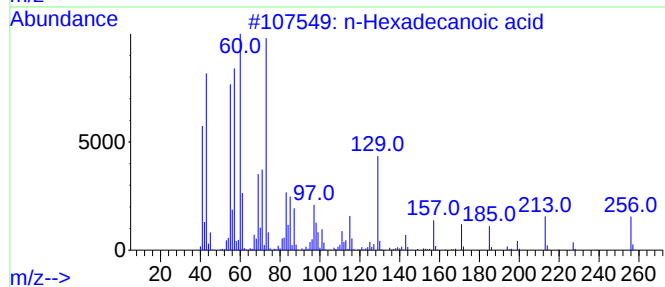
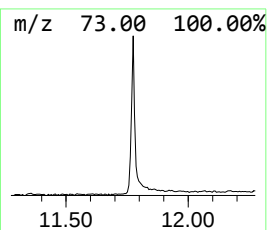
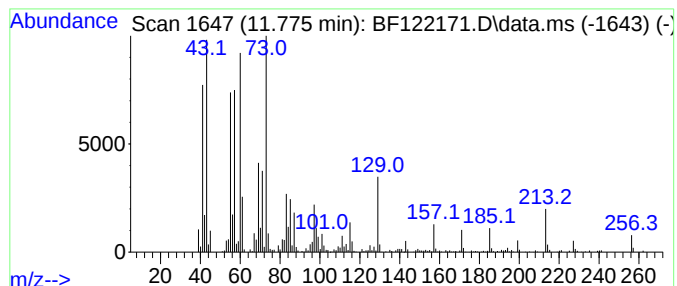
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.775	12.46 ng	587085	Phenanthrene-d10	11.233

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Tridecanoic acid	214	C13H26O2	000638-53-9	94
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	87
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	70
5			Undecanoic acid	186	C11H22O2	000112-37-8	50



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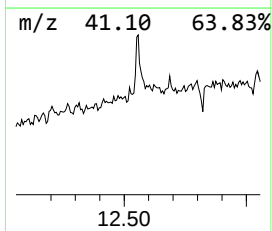
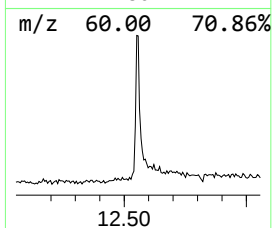
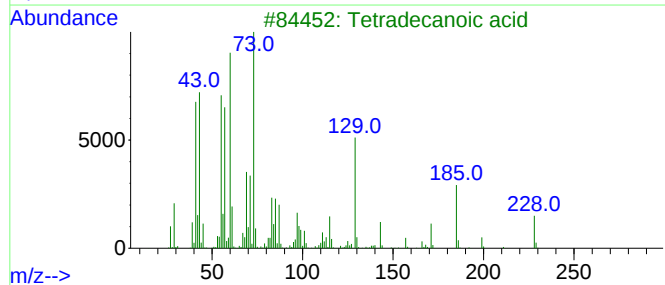
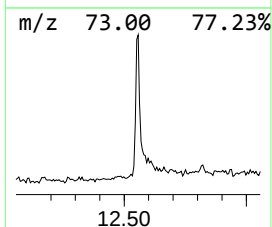
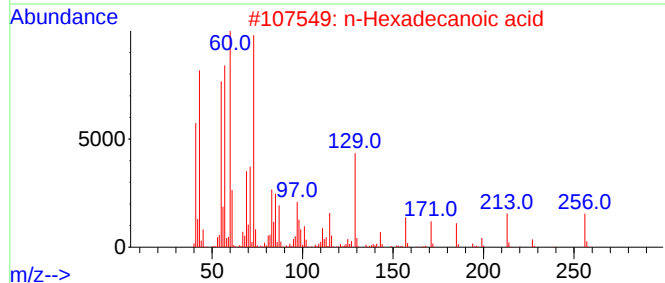
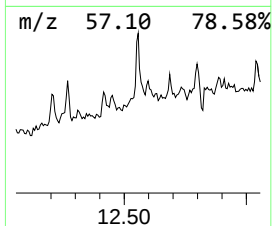
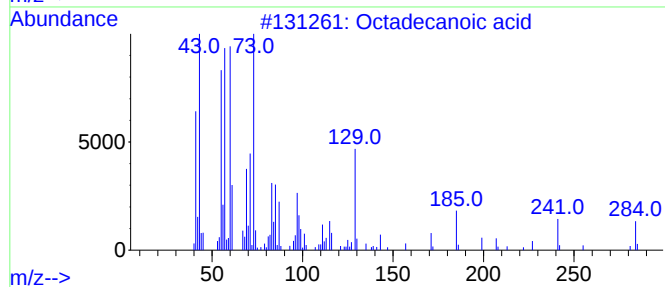
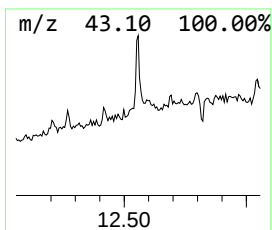
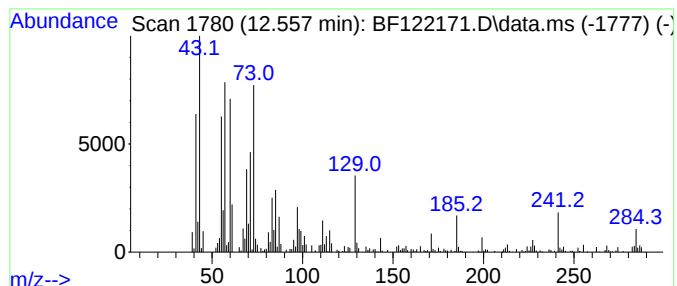
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 3 Octadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.557	3.93 ng	185364	Phenanthrene-d10	11.233

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	68
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	64
4			Tridecanoic acid	214	C13H26O2	000638-53-9	53
5			11-Bromoundecanoic acid	264	C11H21BrO2	002834-05-1	38



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Misc :
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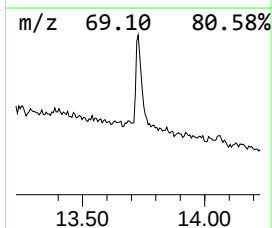
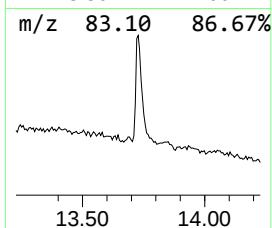
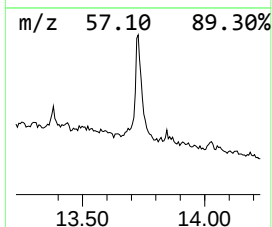
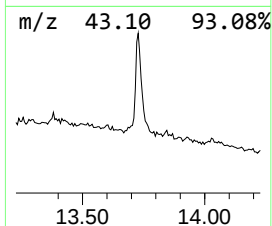
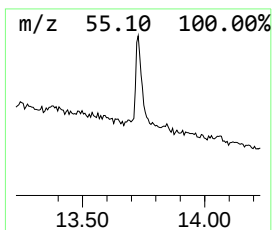
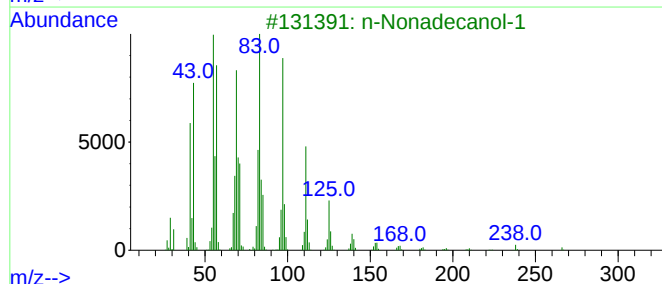
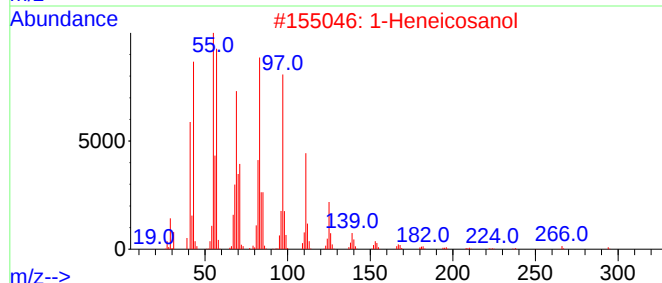
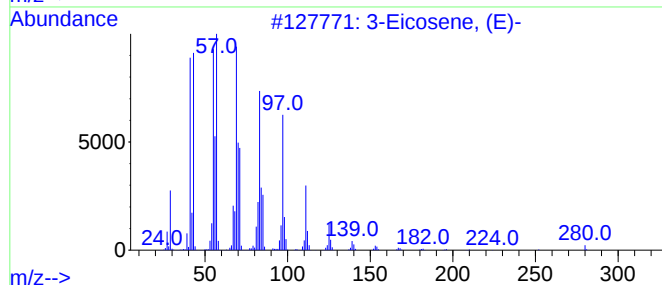
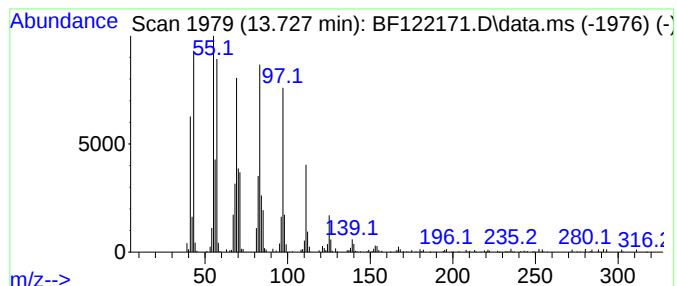
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 4 3-Eicosene, (E)- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD		R.T.	
13.727	18.11 ng	639316	Chrysene-d12		13.880	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	3-Eicosene, (E)-		280	C20H40	074685-33-9	96
2	1-Heneicosanol		312	C21H44O	015594-90-8	95
3	n-Nonadecanol-1		284	C19H40O	001454-84-8	95
4	1-Hexadecanol		242	C16H34O	036653-82-4	91
5	1-Nonadecene		266	C19H38	018435-45-5	91



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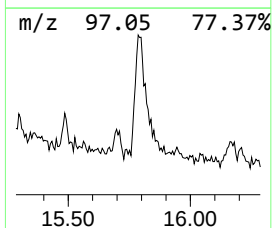
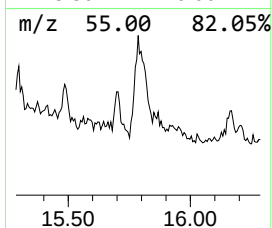
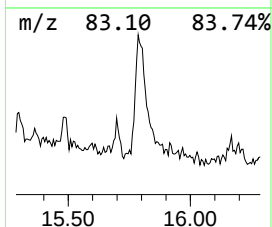
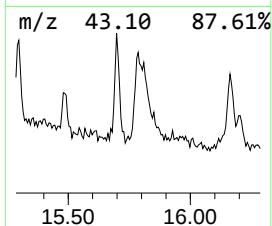
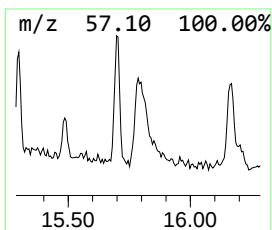
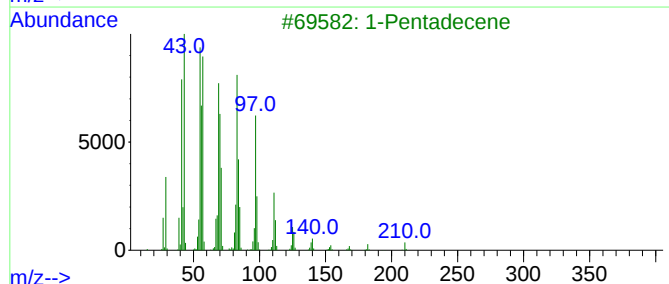
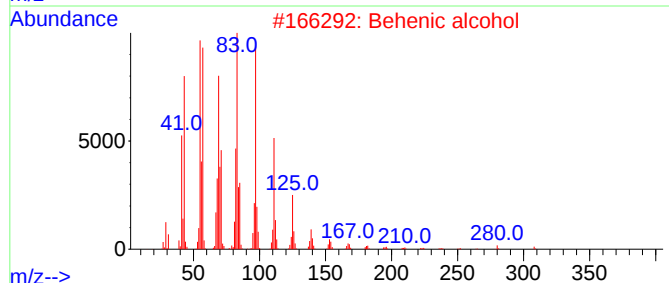
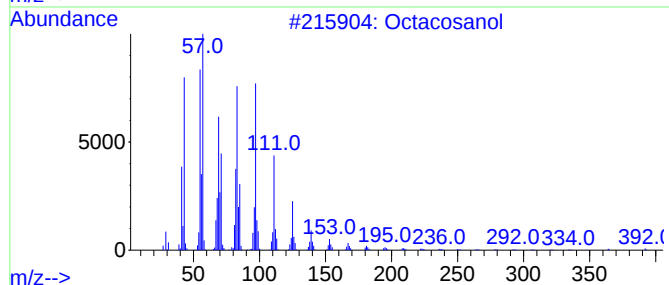
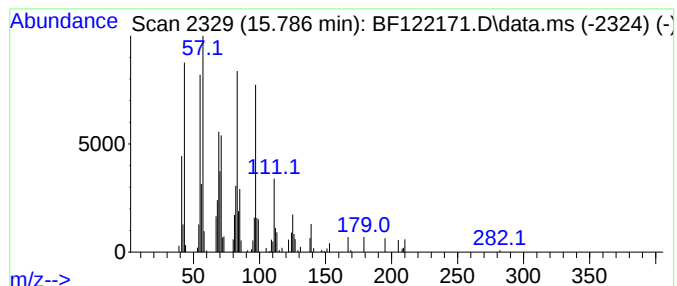
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Peak Number 5 Octacosanol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.786	5.01 ng	175685	Perylene-d12	15.316

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octacosanol	410	C28H58O	000557-61-9	93
2			Behenic alcohol	326	C22H46O	000661-19-8	93
3			1-Pentadecene	210	C15H30	013360-61-7	90
4			Cyclopentadecane	210	C15H30	000295-48-7	86
5			Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	81



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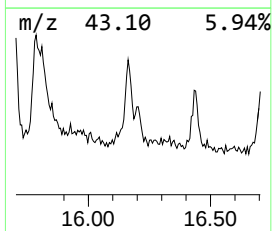
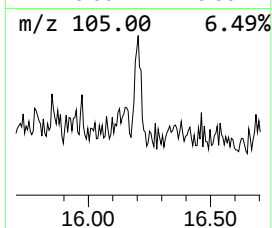
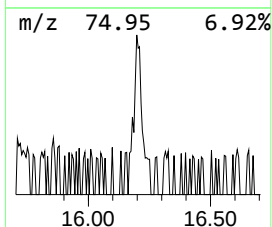
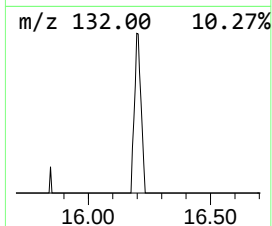
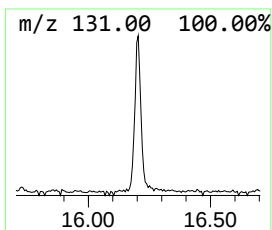
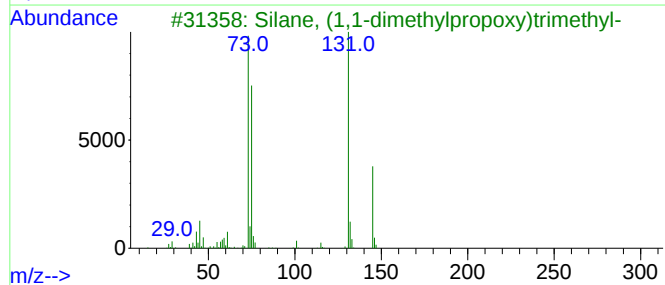
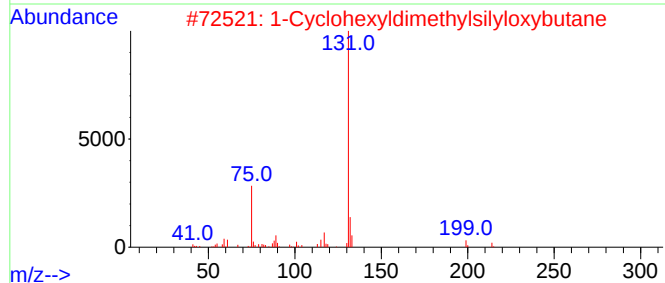
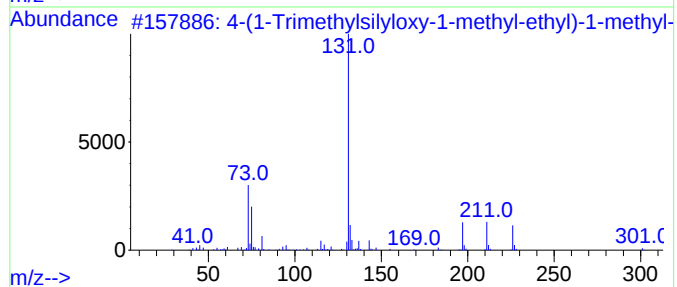
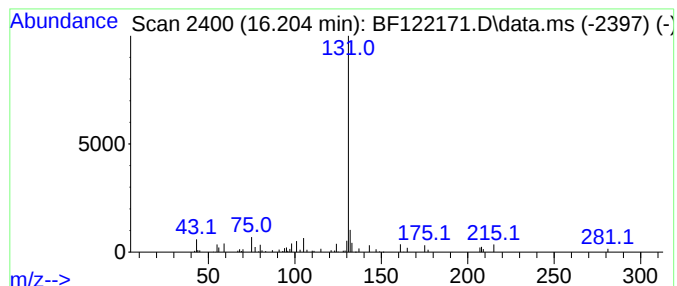
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 4-(1-Trimethylsilyloxy-1-me... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.204	2.00 ng	70289	Perylene-d12	15.316

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			4-(1-Trimethylsilyloxy-1-methyl-...	316	C16H36O2Si2	1000373-06-9	50
2			1-Cyclohexyldimethylsilyloxybutane	214	C12H26OSi	1000281-95-6	39
3			Silane, (1,1-dimethylpropoxy)tri...	160	C8H20OSi	006689-16-3	39
4			2,2-Dimethyl-3-pentanol, trimeth...	188	C10H24OSi	1000364-14-3	39
5			2-Methyl-3-pentanol, trimethylsi...	174	C9H22OSi	1000352-36-6	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102920\
Data File : BF122171.D
Acq On : 29 Oct 2020 18:45
Operator : JU/CG
Sample : L4552-04
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
VW-STONE-B

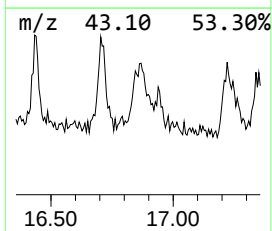
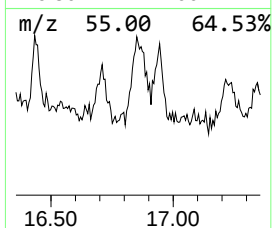
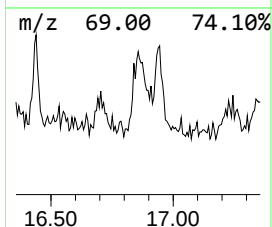
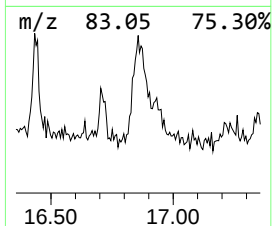
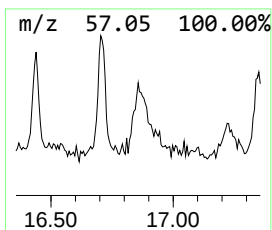
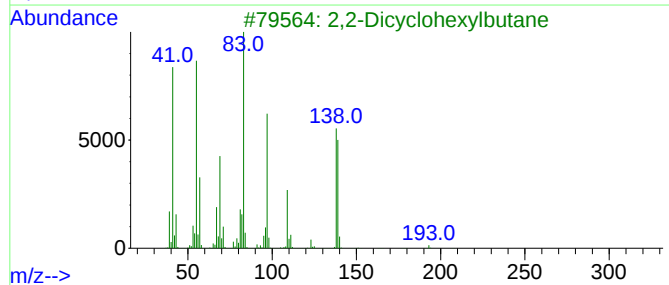
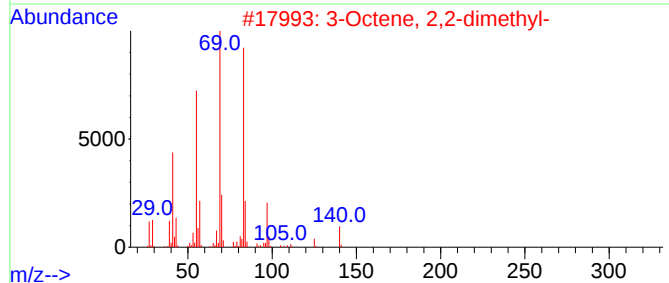
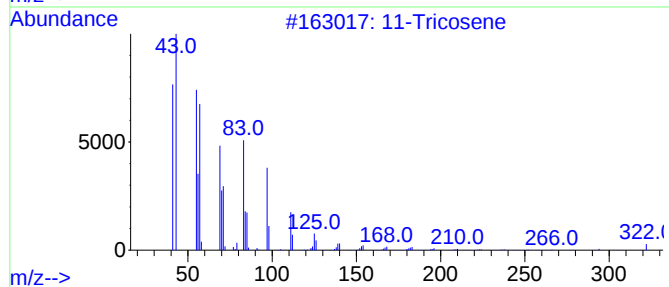
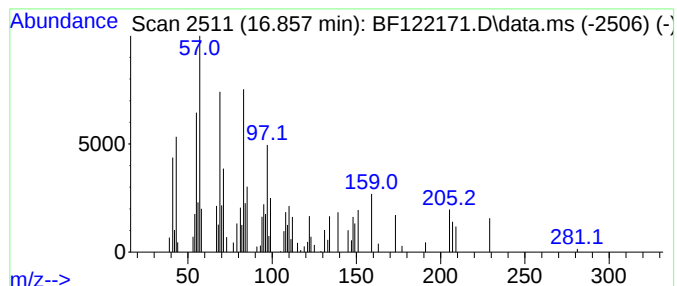
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 11-Tricosene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.857	2.11 ng	74048	Perylene-d12	15.316

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			11-Tricosene	322	C23H46	052078-56-5	50
2			3-Octene, 2,2-dimethyl-	140	C10H20	086869-76-3	38
3			2,2-Dicyclohexylbutane	222	C16H30	054890-02-7	22
4			Cyclohexanone, 3-ethyl-	126	C8H14O	022461-89-8	22
5			5-Hexen-2-one, 5-methyl-	112	C7H12O	003240-09-3	22



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102920\
Data File : BF122171.D
Acq On : 29 Oct 2020 18:45
Operator : JU/CG
Sample : L4552-04
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
VW-STONE-B

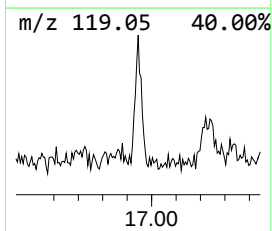
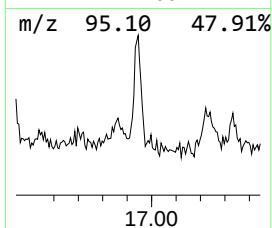
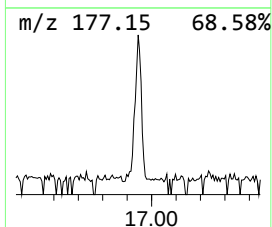
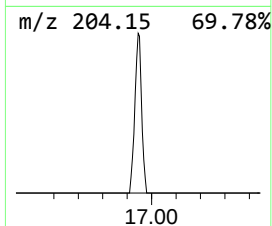
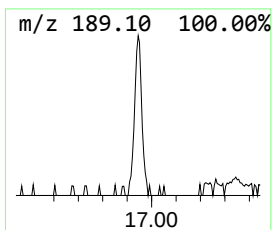
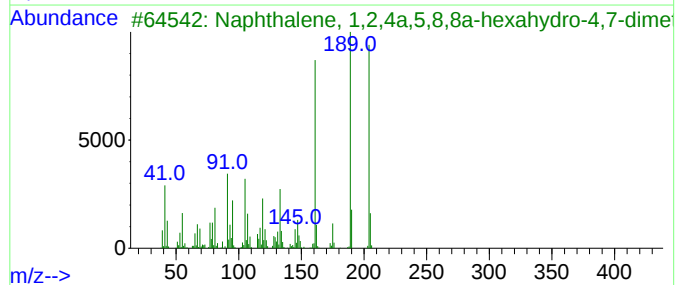
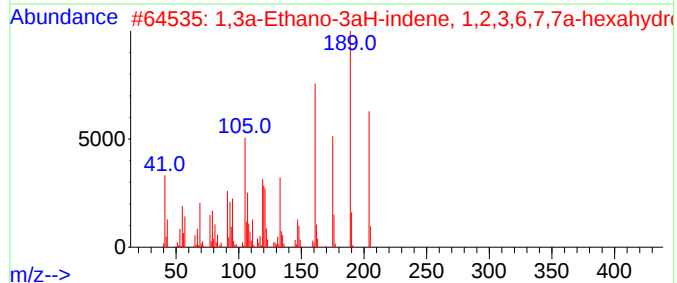
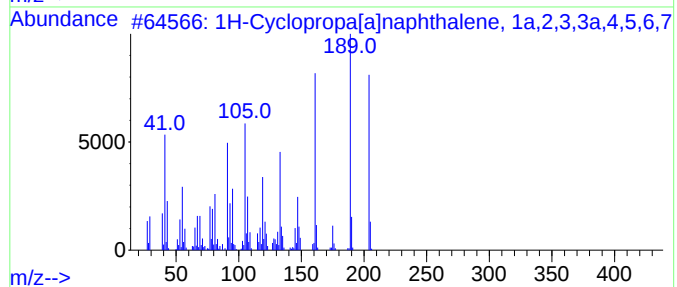
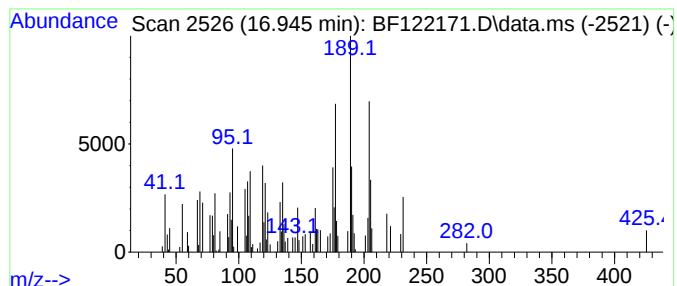
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 8 unknown16.945 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.945	4.58 ng	160683	Perylene-d12	15.316

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1H-Cyclopropa[a]naphthalene, 1a,...	204	C15H24	000489-29-2	46
2			1,3a-Ethano-3aH-indene, 1,2,3,6,...	204	C15H24	004545-68-0	43
3			Naphthalene, 1,2,4a,5,8,8a-hexah...	204	C15H24	005951-61-1	38
4			1,4-Dimethyl-8-isopropylidenetri...	204	C15H24	1000140-07-7	25
5			10-epi-.gamma.-Eudesmol	222	C15H26O	015051-81-7	25



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102920\
Data File : BF122171.D
Acq On : 29 Oct 2020 18:45
Operator : JU/CG
Sample : L4552-04
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
VW-STONE-B

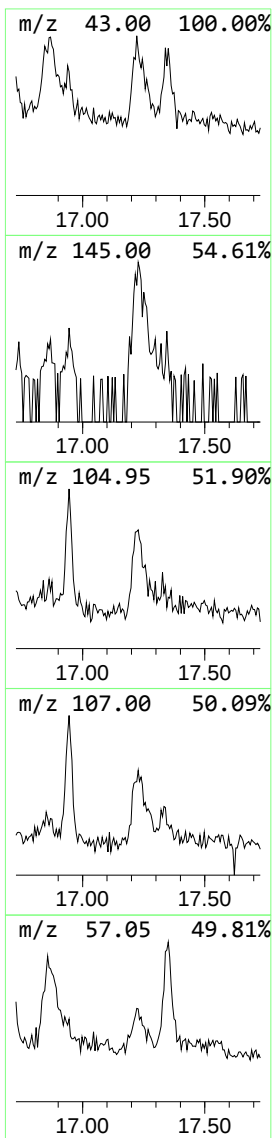
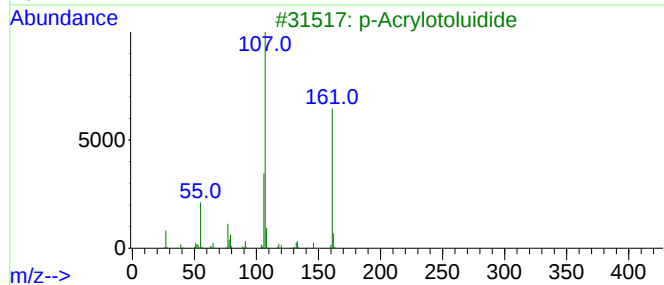
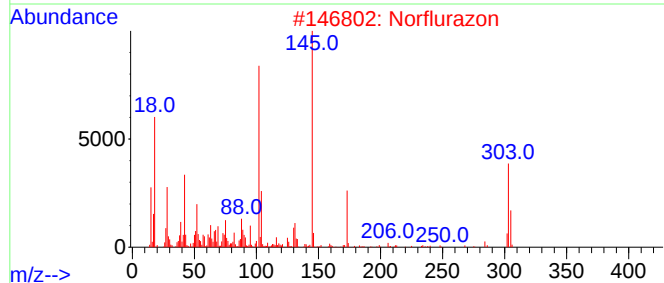
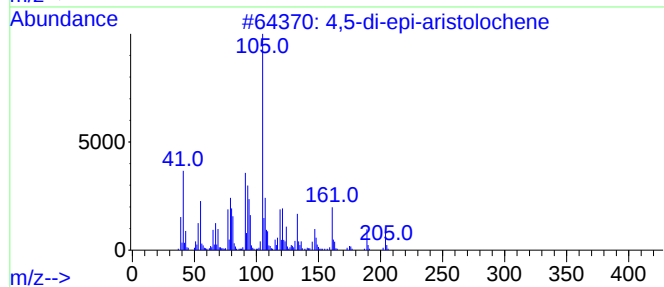
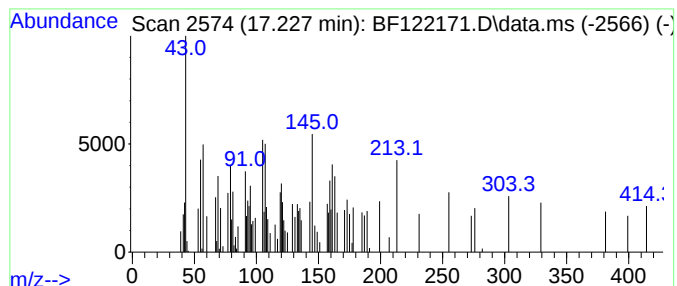
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 9 unknown17.227 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.227	3.86 ng	135556	Perylene-d12	15.316

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			4,5-di-epi-aristolochene	204	C15H24	1000374-17-1	10
2			Norflurazon	303	C12H9ClF3N3O	027314-13-2	9
3			p-Acrylotoluidide	161	C10H11NO	007766-36-1	9
4			5,16-Pregnenolone oxime	329	C21H31NO2	001045-71-2	9
5			1H-Cycloprop[e]azulen-4-ol, deca...	222	C15H26O	000552-02-3	9



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102920\
Data File : BF122171.D
Acq On : 29 Oct 2020 18:45
Operator : JU/CG
Sample : L4552-04
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
VW-STONE-B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101220.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Phthalic anhydride	8.810	4.5	ng	174225	2	7.998	780446	20.0
n-Hexadecanoic ...	11.775	12.5	ng	587085	4	11.233	942498	20.0
Octadecanoic acid	12.557	3.9	ng	185364	4	11.233	942498	20.0
3-Eicosene, (E)-	13.727	18.1	ng	639316	5	13.880	706056	20.0
Octacosanol	15.786	5.0	ng	175685	6	15.316	701752	20.0
4-(1-Trimethyls...	16.204	2.0	ng	70289	6	15.316	701752	20.0
11-Tricosene	16.857	2.1	ng	74048	6	15.316	701752	20.0
unknown16.945	16.945	4.6	ng	160683	6	15.316	701752	20.0
unknown17.227	17.227	3.9	ng	135556	6	15.316	701752	20.0