

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF062124\
 Data File : BF138290.D
 Acq On : 21 Jun 2024 17:32
 Operator : CG\JU
 Sample : P2977-12
 Misc :
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 OSTL-B6

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-BF061224.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF138290.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.175	9	15	21	rVB	2799880	3463791	99.54%	9.737%
2	5.069	503	507	508	rBV	46484	42605	1.22%	0.120%
3	5.098	508	512	520	rVB	404315	445761	12.81%	1.253%
4	5.504	576	581	584	rBV	3379086	3237048	93.02%	9.100%
5	5.828	631	636	641	rBV	60622	54553	1.57%	0.153%
6	6.510	747	752	755	rBV	3268562	3182705	91.46%	8.947%
7	6.881	812	815	819	rVB	2024057	1677116	48.20%	4.715%
8	7.439	906	910	914	rBV	2218688	2090330	60.07%	5.876%
9	7.692	950	953	957	rBV	100988	81702	2.35%	0.230%
10	7.969	997	1000	1008	rVB	57401	48382	1.39%	0.136%
11	8.163	1029	1033	1036	rBV	2785701	2203866	63.33%	6.195%
12	8.475	1082	1086	1097	rBV	120701	141473	4.07%	0.398%
13	9.239	1212	1216	1219	rBV	4309421	3479797	100.00%	9.782%
14	9.833	1314	1317	1325	rBV	217820	206501	5.93%	0.580%
15	9.916	1328	1331	1335	rBV	2738313	2329132	66.93%	6.547%
16	10.016	1343	1348	1357	rBV	642206	792163	22.76%	2.227%
17	10.704	1461	1465	1468	rBV	1888457	1563854	44.94%	4.396%
18	11.404	1580	1584	1587	rBV	2215140	1871131	53.77%	5.260%
19	11.927	1670	1673	1678	rBV2	185895	182006	5.23%	0.512%
20	12.610	1786	1789	1793	rBV	141730	128515	3.69%	0.361%
21	12.839	1823	1828	1834	rVB	121135	126028	3.62%	0.354%
22	12.986	1849	1853	1856	rBV	3311617	2693080	77.39%	7.571%
23	13.557	1940	1950	1954	rBV10	15302	41291	1.19%	0.116%
24	13.892	2003	2007	2025	rBV8	69555	273352	7.86%	0.768%
25	14.039	2027	2032	2035	rVV	1763426	1601663	46.03%	4.502%
26	14.062	2035	2036	2044	rVB	97603	75708	2.18%	0.213%
27	14.509	2109	2112	2115	rBV	57552	48605	1.40%	0.137%
28	14.898	2174	2178	2182	rBV	146606	154573	4.44%	0.435%
29	14.968	2186	2190	2195	rVV	93422	100663	2.89%	0.283%
30	15.080	2205	2209	2212	rBV	71654	116225	3.34%	0.327%
31	15.162	2219	2223	2226	rBV	84910	95397	2.74%	0.268%
32	15.380	2257	2260	2266	rVB	42948	54125	1.56%	0.152%
33	15.445	2267	2271	2276	rVV	48221	61862	1.78%	0.174%
34	15.509	2277	2282	2294	rVB	1122570	1430172	41.10%	4.020%
35	15.751	2320	2323	2329	rVB	56016	76905	2.21%	0.216%
36	15.992	2360	2364	2369	rVB	62918	89335	2.57%	0.251%

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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-BF061224.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	16.803	2498	2502	2510	rVB3	40239	76716	2.20%	0.216%
38	17.174	2559	2565	2573	rBV2	175629	327766	9.42%	0.921%
39	17.350	2589	2595	2603	rVB2	104241	220372	6.33%	0.619%
40	18.174	2729	2735	2745	rVB7	71782	213132	6.12%	0.599%
41	18.692	2815	2823	2832	rVB3	162470	473918	13.62%	1.332%

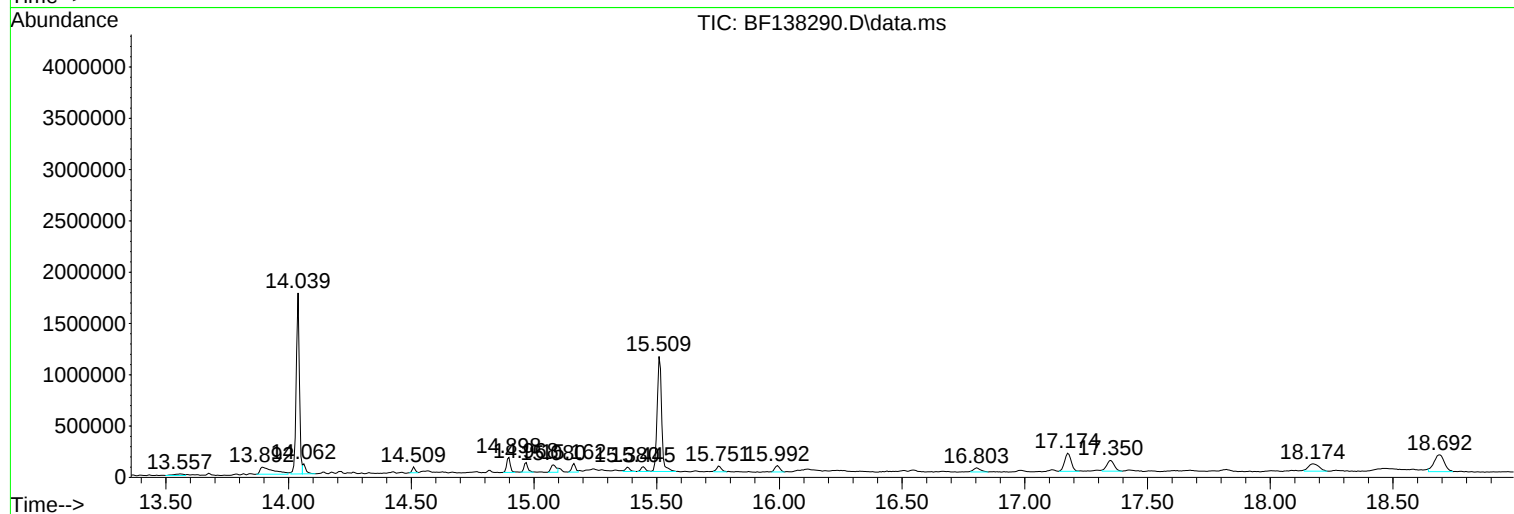
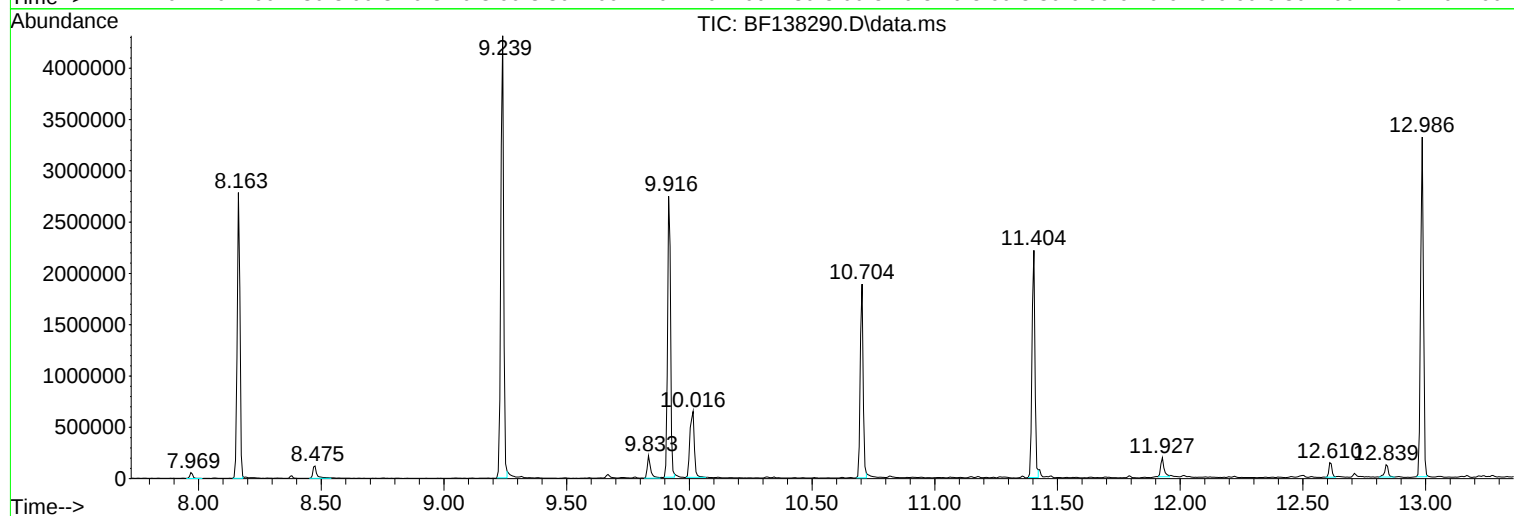
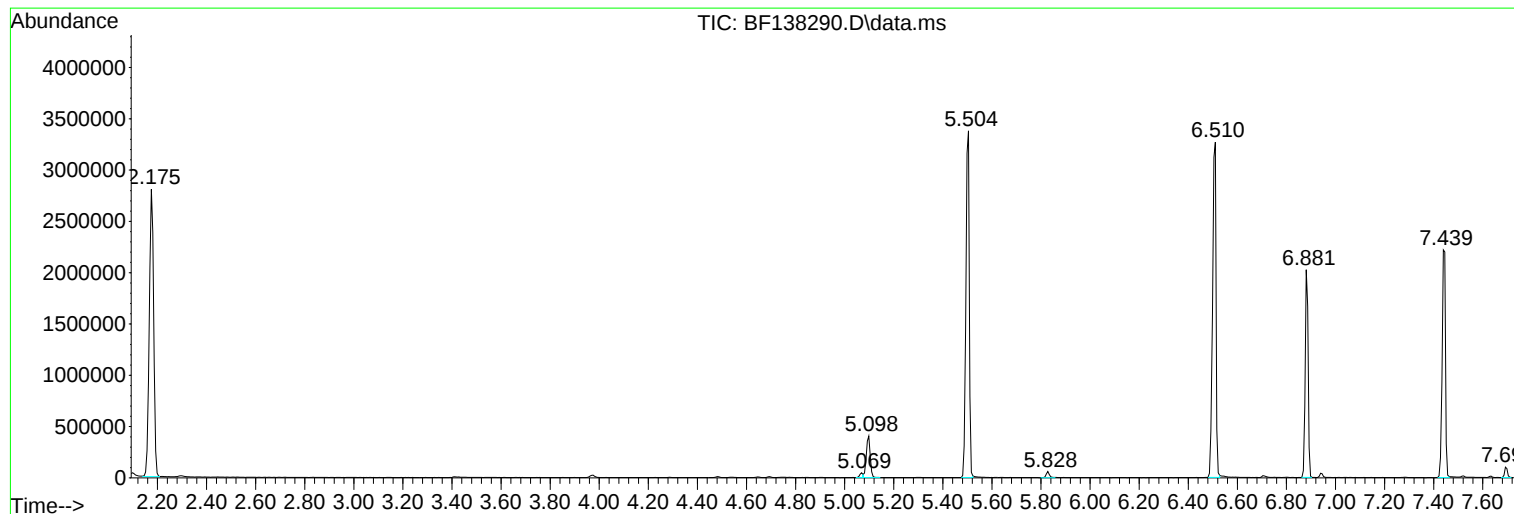
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF061224.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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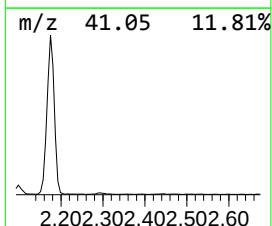
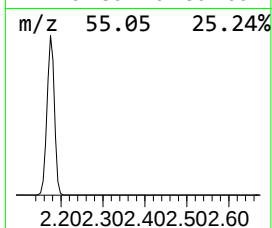
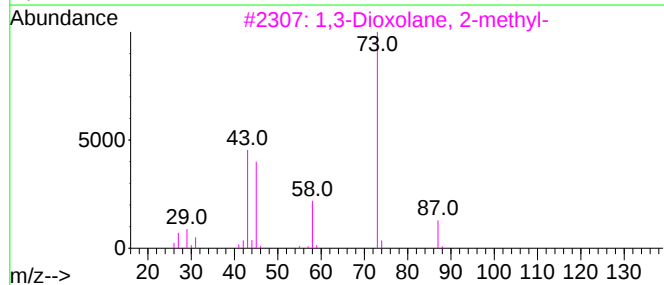
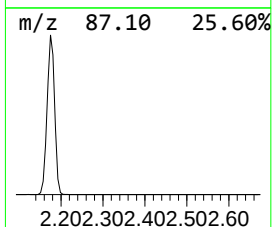
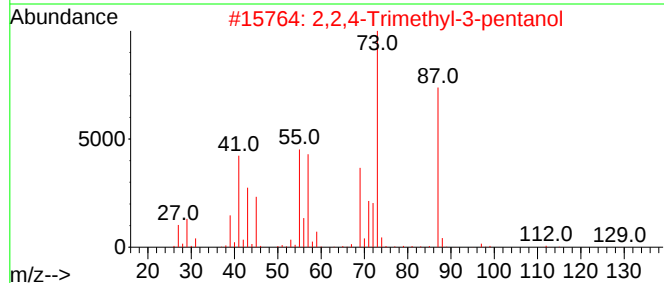
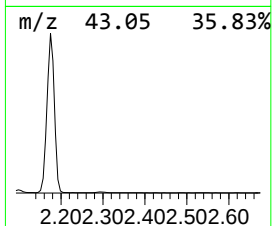
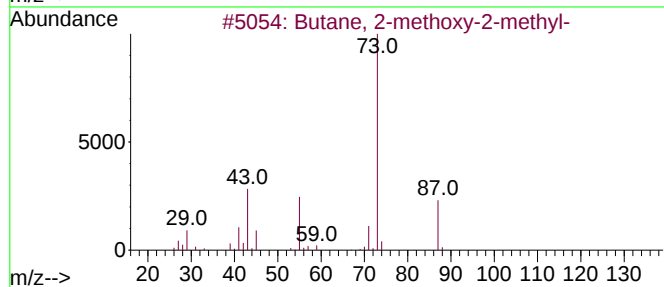
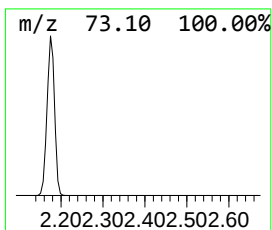
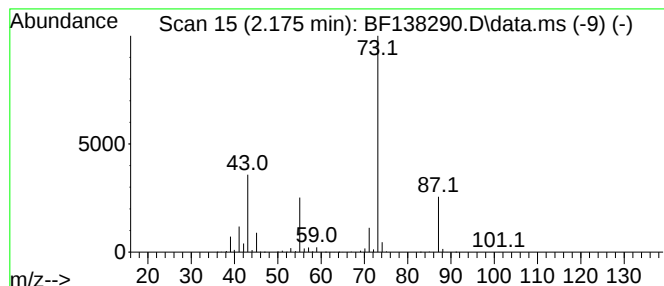
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF061224.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
2.175	41.31 ng	3463790	1,4-Dichlorobenzene-d4	6.881

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
4			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	23
5			Silane, tetramethyl-	88	C4H12Si	000075-76-3	17



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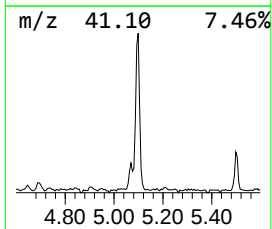
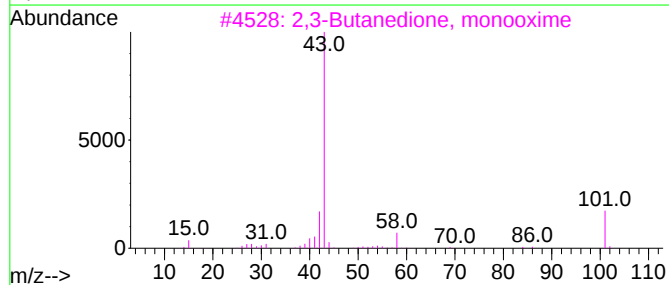
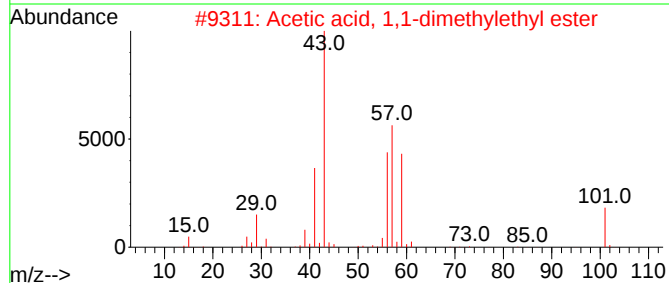
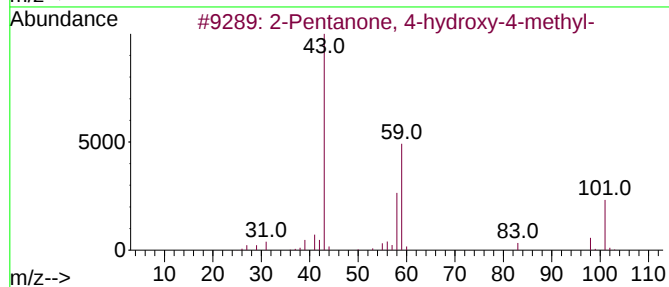
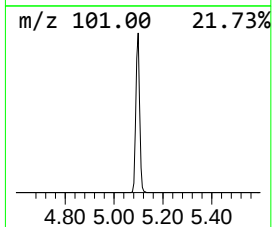
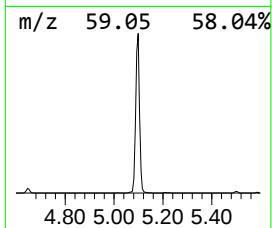
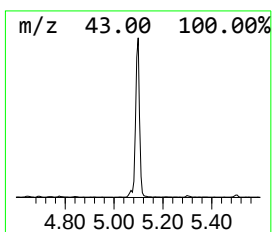
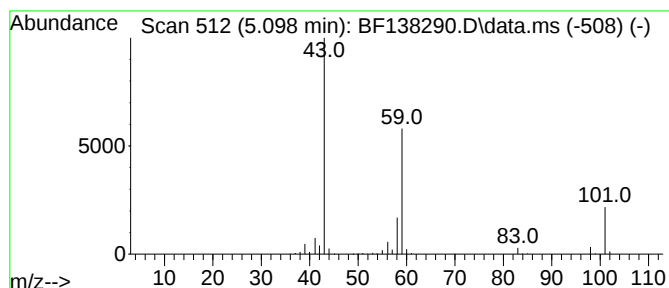
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.098	5.32 ng	445761	1,4-Dichlorobenzene-d4	6.881

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25
4			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
5			(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9



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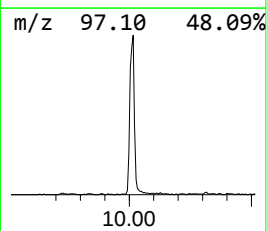
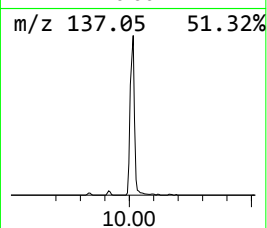
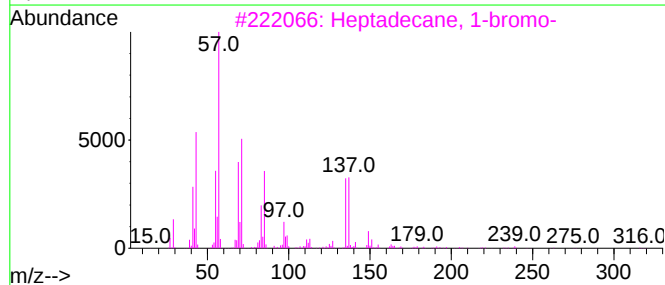
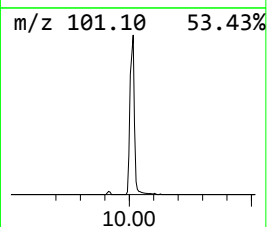
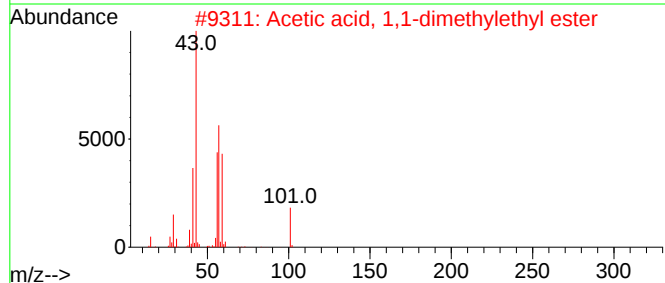
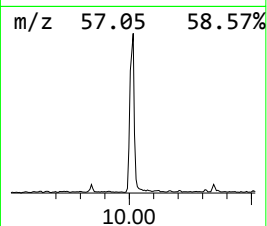
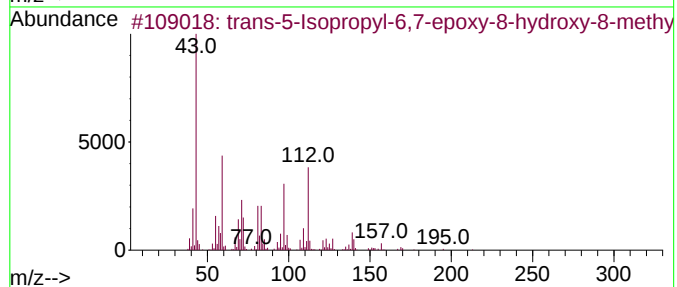
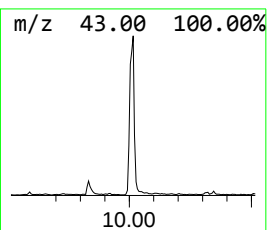
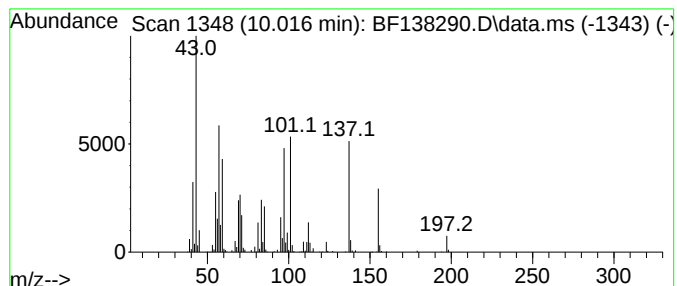
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown10.016 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.016	6.80 ng	792163	Acenaphthene-d10	9.916

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			trans-5-Isopropyl-6,7-epoxy-8-hy...	228	C13H24O3	058002-07-6	16
2			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	10
3			Heptadecane, 1-bromo-	318	C17H35Br	003508-00-7	10
4			Benzoic acid, 2-amino-4-fluoro-	155	C7H6FN02	000446-32-2	10
5			Acetoxyacetic acid, 5-tetradecyl...	314	C18H34O4	1000308-81-0	10



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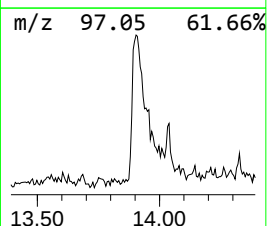
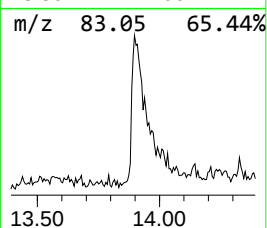
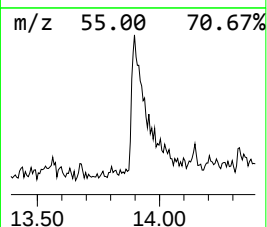
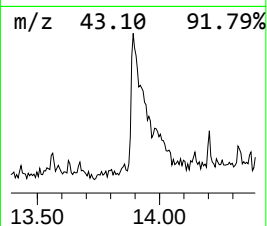
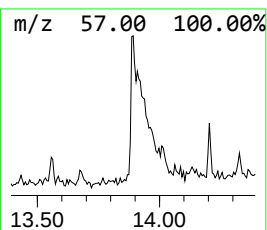
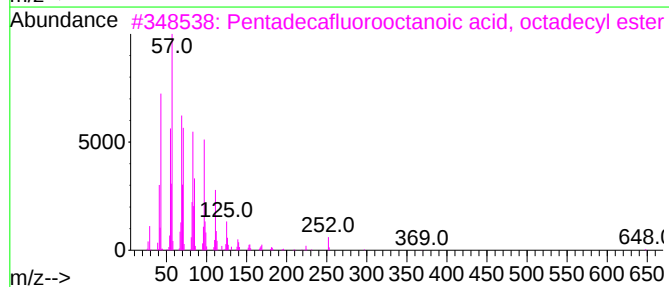
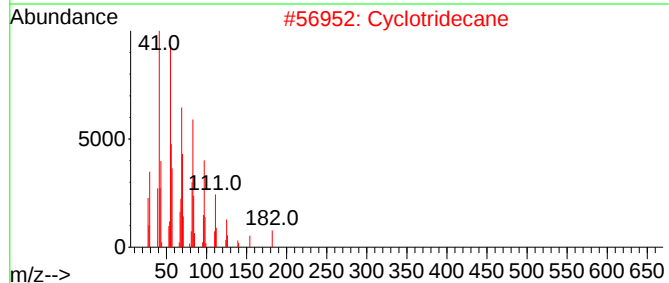
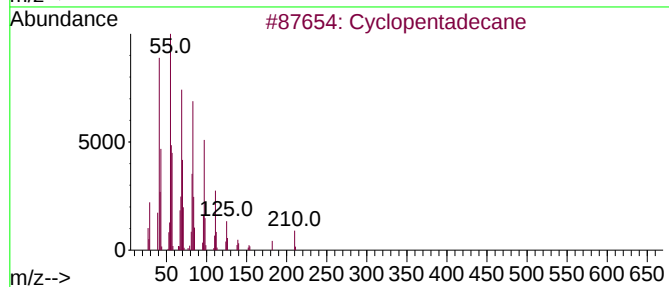
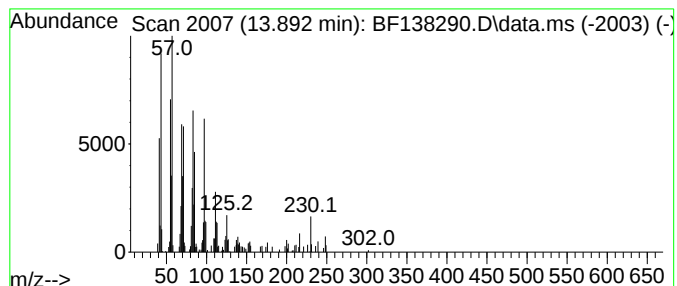
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 Cyclopentadecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.892	3.41 ng	273352	Chrysene-d12	14.039

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopentadecane	210	C15H30	000295-48-7	96
2			Cyclotridecane	182	C13H26	000295-02-3	95
3			Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	93
4			2-Hepten-4-one, 6-hydroxy-2-meth...	236	C15H24O2	038043-98-0	90
5			Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	90



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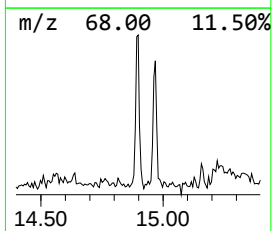
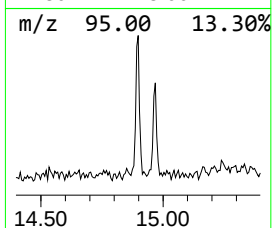
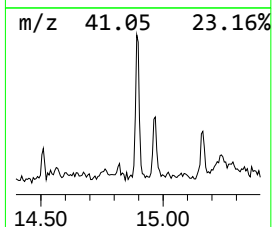
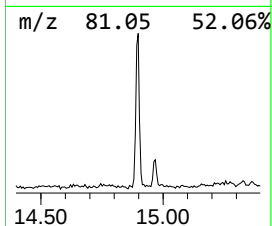
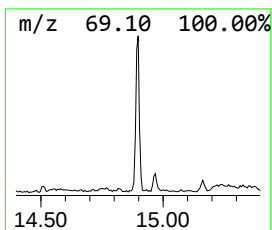
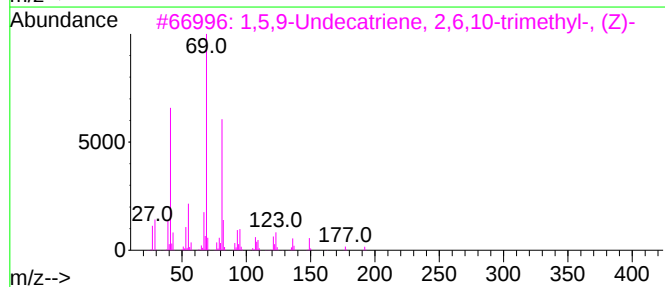
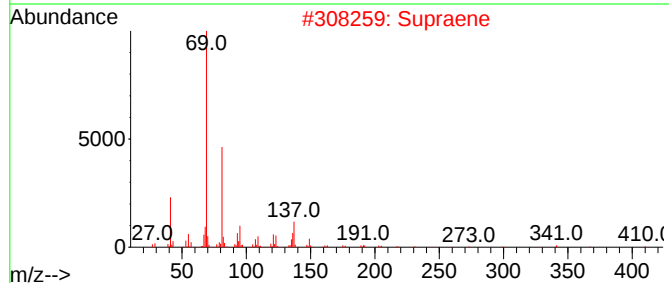
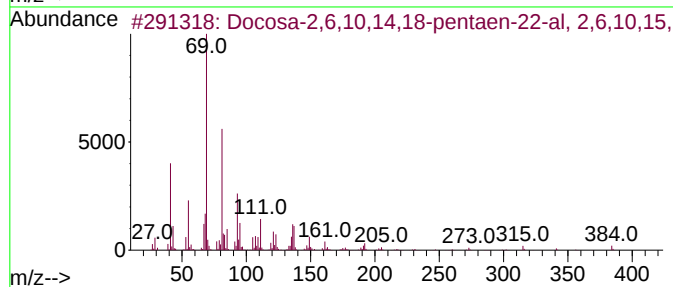
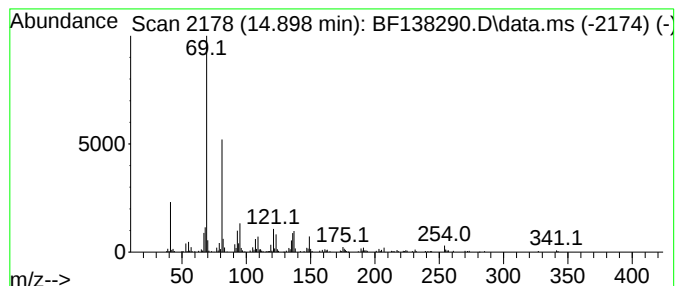
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Docosa-2,6,10,14,18-pentaen... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.898	2.16 ng	154573	Perylene-d12	15.509

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Docosa-2,6,10,14,18-pentaen-22-a...	384	C27H44O	1000163-04-7	90		
2	Supraene	410	C30H50	007683-64-9	87		
3	1,5,9-Undecatriene, 2,6,10-trime...	192	C14H24	062951-96-6	83		
4	3,7,11-Trimethyl-dodeca-2,6,10-t...	236	C15H24O2	007548-13-2	78		
5	1,6,10-Dodecatrien-3-ol, 3,7,11-...	222	C15H26O	007212-44-4	59		



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF062124\
Data File : BF138290.D
Acq On : 21 Jun 2024 17:32
Operator : CG\JU
Sample : P2977-12
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
OSTL-B6

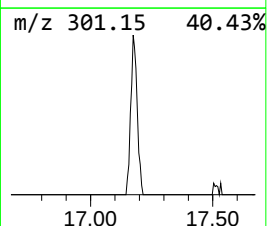
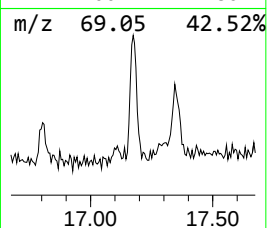
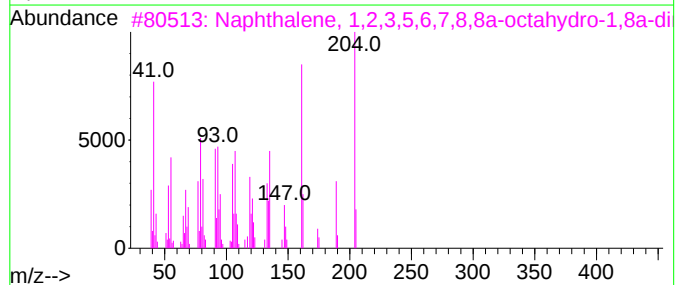
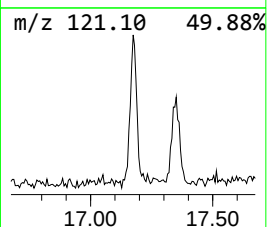
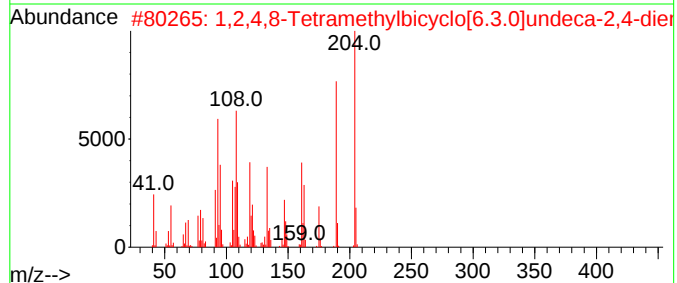
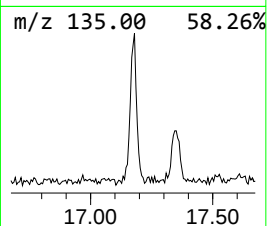
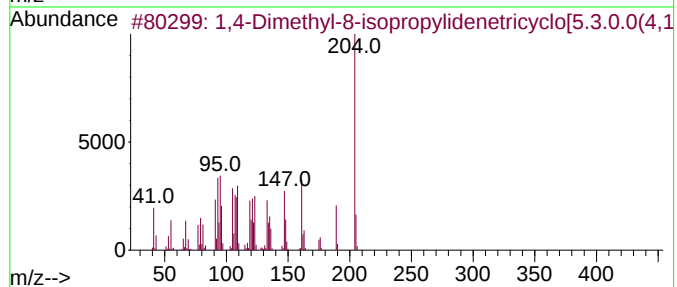
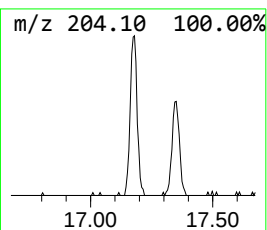
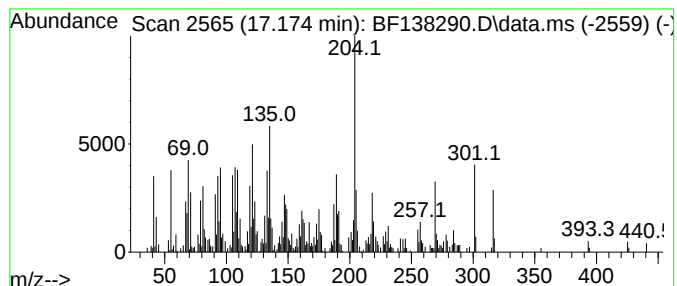
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 1,4-Dimethyl-8-isopropylide... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.174	4.58 ng	327766	Perylene-d12	15.509

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,4-Dimethyl-8-isopropylidenetri...	204	C15H24	1010140-07-7	53
2			1,2,4,8-Tetramethylbicyclo[6.3.0...	204	C15H24	137235-51-9	45
3			Naphthalene, 1,2,3,5,6,7,8,8a-oc...	204	C15H24	004630-07-3	43
4			1-(4-(2-ethoxybenzyl)piperazin-1...	316	C15H19F3N2O2	1000455-08-1	38
5			Guaia-3,9-diene	204	C15H24	000489-83-8	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF062124\
Data File : BF138290.D
Acq On : 21 Jun 2024 17:32
Operator : CG\JU
Sample : P2977-12
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
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ClientSampleId :
OSTL-B6

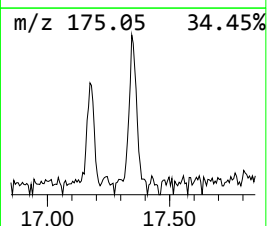
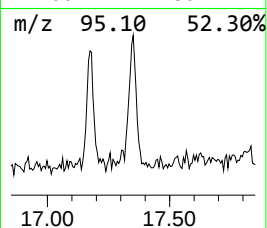
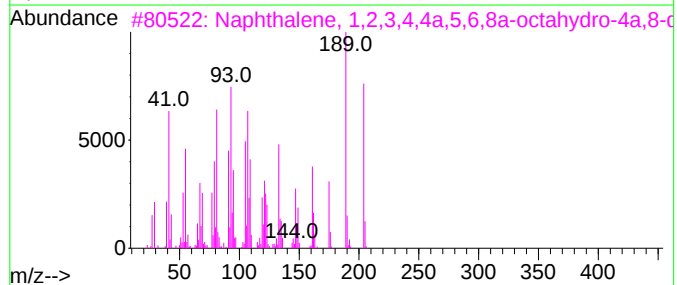
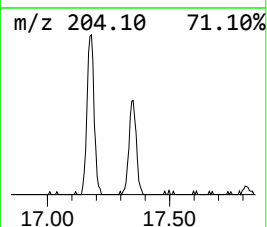
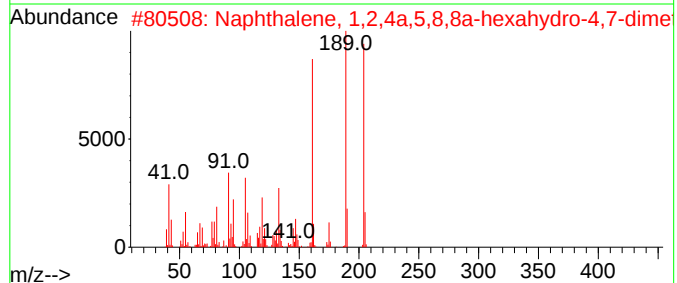
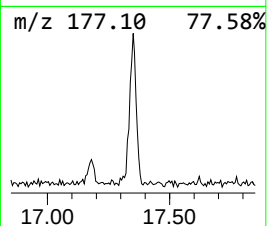
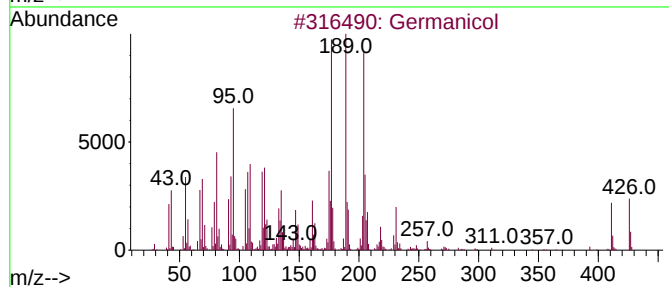
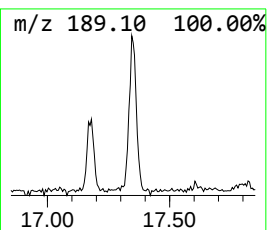
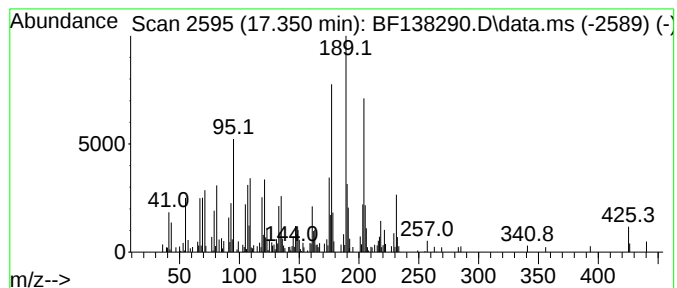
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Germanicol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.351	3.08 ng	220372	Perylene-d12	15.509

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Germanicol	426	C30H50O	000465-02-1	68
2			Naphthalene, 1,2,4a,5,8,8a-hexah...	204	C15H24	005951-61-1	46
3			Naphthalene, 1,2,3,4,4a,5,6,8a-o...	204	C15H24	000473-13-2	38
4			1H-Cyclopropa[a]naphthalene, 1a,...	204	C15H24	000489-29-2	38
5			1-(4,5-Dimethyl-6H-thiopyran-2-y...	204	C9H10F2OS	1000318-25-0	30



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF062124\
Data File : BF138290.D
Acq On : 21 Jun 2024 17:32
Operator : CG\JU
Sample : P2977-12
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
OSTL-B6

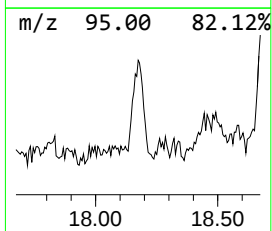
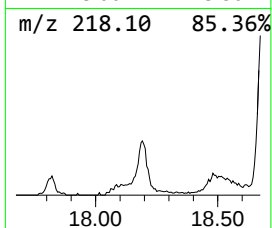
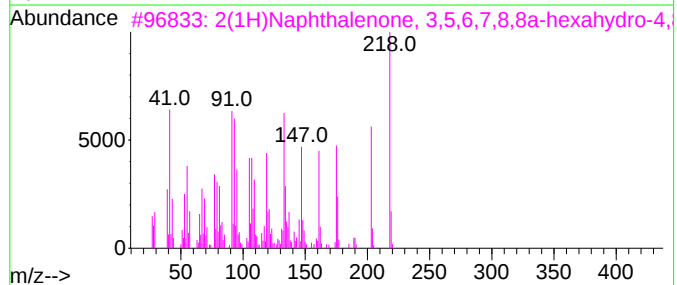
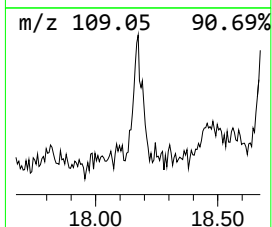
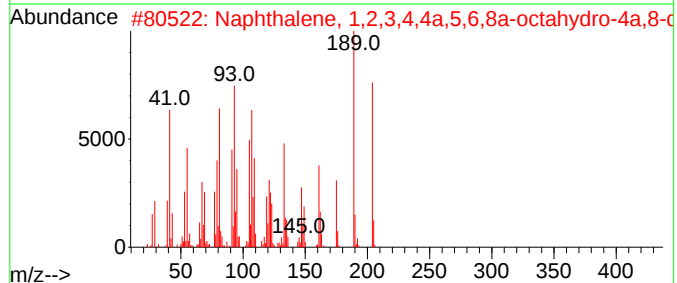
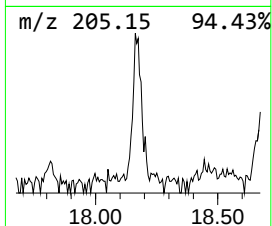
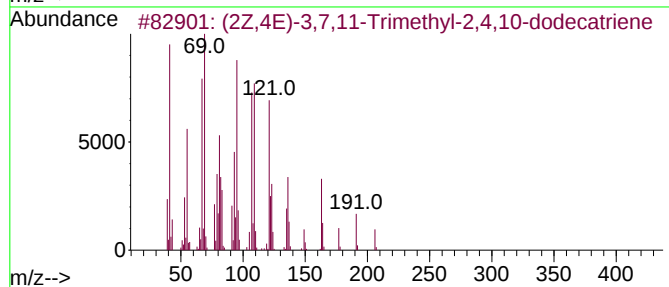
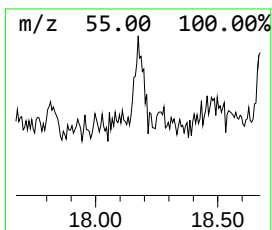
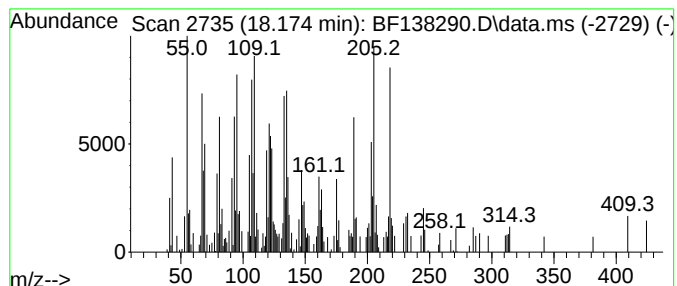
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 (2Z,4E)-3,7,11-Trimethyl-2,... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.174	2.98 ng	213132	Perylene-d12	15.509

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			(2Z,4E)-3,7,11-Trimethyl-2,4,10-...	206	C15H26	172549-29-0	89
2			Naphthalene, 1,2,3,4,4a,5,6,8a-o...	204	C15H24	000473-13-2	58
3			2(1H)Naphthalenone, 3,5,6,7,8,8a...	218	C15H22O	1000188-66-5	47
4			Boron, 1,5-cyclooctanediyl(2,4-p...	218	C13H23BN2	136704-99-9	42
5			1-Propyl-2,2-bis(phenylthio)cycl...	314	C19H22S2	122732-89-2	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF062124\
Data File : BF138290.D
Acq On : 21 Jun 2024 17:32
Operator : CG\JU
Sample : P2977-12
Misc :
ALS Vial : 14 Sample Multiplier: 1

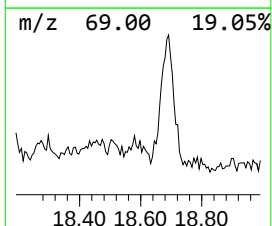
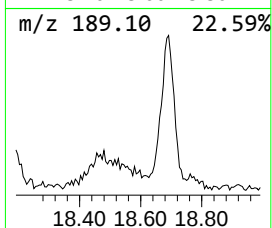
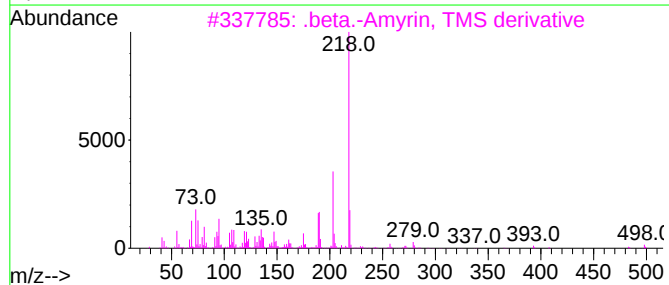
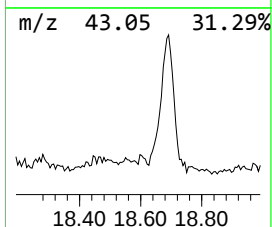
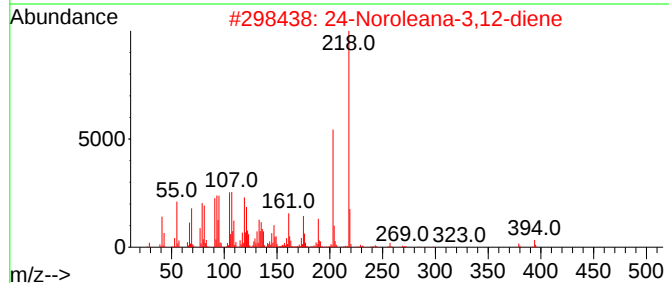
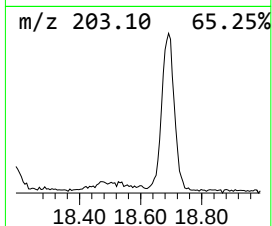
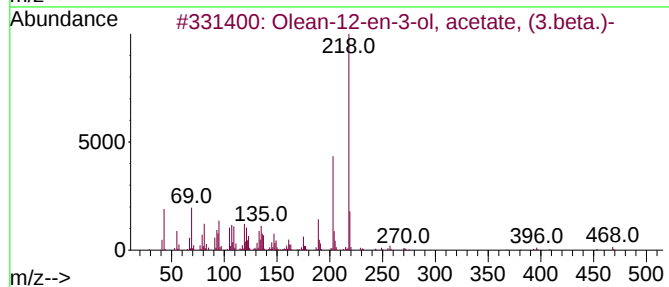
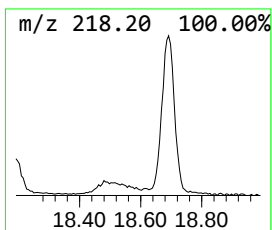
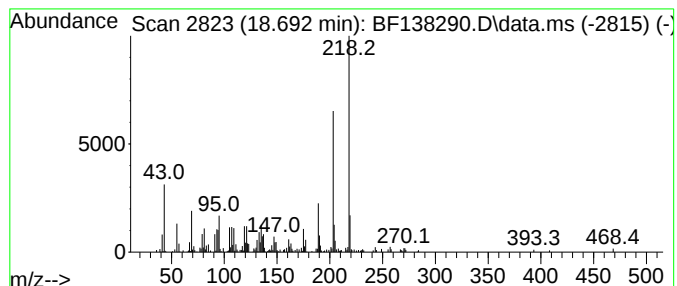
Instrument :
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ClientSampleId :
OSTL-B6

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF061224.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Olean-12-en-3-ol, acetate, ... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.	
18.692	6.63 ng	473918	Perylene-d12	15.509	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Olean-12-en-3-ol, acetate, (3.be...	468	C32H52O2	001616-93-9	99
2	24-Noroleana-3,12-diene	394	C29H46	201358-24-9	86
3	.beta.-Amyrin, TMS derivative	498	C33H58OSi	001721-67-1	72
4	.beta.-Amyrin	426	C30H50O	000559-70-6	68
5	3-Methoxy-6,7,8,9-tetrahydro-dib...	218	C13H14O3	1000186-57-9	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF062124\
Data File : BF138290.D
Acq On : 21 Jun 2024 17:32
Operator : CG\JU
Sample : P2977-12
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
OSTL-B6

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF061224.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
Butane, 2-metho...	2.175	41.3	ng	3463790	1	6.881	1677120	20.0
2-Pentanone, 4-...	5.098	5.3	ng	445761	1	6.881	1677120	20.0
unknown10.016	10.016	6.8	ng	792163	3	9.916	2329130	20.0
Cyclopentadecane	13.892	3.4	ng	273352	5	14.039	1601660	20.0
Docosa-2,6,10,1...	14.898	2.2	ng	154573	6	15.509	1430170	20.0
1,4-Dimethyl-8-...	17.174	4.6	ng	327766	6	15.509	1430170	20.0
Germanicol	17.351	3.1	ng	220372	6	15.509	1430170	20.0
(2Z,4E)-3,7,11-...	18.174	3.0	ng	213132	6	15.509	1430170	20.0
Olean-12-en-3-o...	18.692	6.6	ng	473918	6	15.509	1430170	20.0