

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF010324\
 Data File : BF136919.D
 Acq On : 03 Jan 2024 21:22
 Operator : CG\JU
 Sample : 05900-01
 Misc :
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 GHL-SS-54

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-BF122023.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF136919.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.169	11	14	22	rVB	13068	18573	1.24%	0.175%
2	5.022	495	499	509	rVB	31422	44981	3.00%	0.424%
3	5.428	564	568	579	rBV	1504908	1374037	91.63%	12.966%
4	6.428	734	738	741	rBV	1389833	1334472	88.99%	12.592%
5	6.781	794	798	801	rBV	451492	345442	23.04%	3.260%
6	7.345	889	894	897	rBV	1006001	890103	59.36%	8.399%
7	8.057	1011	1015	1018	rBV	577760	446319	29.76%	4.212%
8	9.133	1194	1198	1201	rBV	1908435	1499582	100.00%	14.151%
9	9.181	1204	1206	1209	rVB2	29587	25764	1.72%	0.243%
10	9.245	1214	1217	1223	rVB4	24909	25868	1.73%	0.244%
11	9.810	1310	1313	1317	rBV	563896	477483	31.84%	4.506%
12	10.604	1444	1448	1459	rVB	868949	801874	53.47%	7.567%
13	10.733	1464	1470	1473	rVB	22893	27014	1.80%	0.255%
14	11.075	1526	1528	1531	rVB	32525	25246	1.68%	0.238%
15	11.304	1563	1567	1570	rBV	526669	415326	27.70%	3.919%
16	11.839	1654	1658	1669	rBV	220271	235821	15.73%	2.225%
17	11.992	1681	1684	1689	rBV4	14541	18605	1.24%	0.176%
18	12.398	1750	1753	1760	rVB3	13193	19346	1.29%	0.183%
19	12.551	1774	1779	1786	rBV7	18302	42714	2.85%	0.403%
20	12.627	1789	1792	1802	rVV2	68336	90629	6.04%	0.855%
21	12.898	1834	1838	1842	rBV	1208576	1010716	67.40%	9.537%
22	13.763	1979	1985	1990	rBV	102407	100910	6.73%	0.952%
23	13.839	1994	1998	2009	rVB6	40193	99925	6.66%	0.943%
24	13.963	2015	2019	2024	rVB	366558	340072	22.68%	3.209%
25	14.092	2037	2041	2044	rBV	57681	55278	3.69%	0.522%
26	14.127	2044	2047	2050	rVV	115057	107186	7.15%	1.011%
27	14.157	2050	2052	2054	rVV	34915	30553	2.04%	0.288%
28	14.180	2054	2056	2060	rVB	42695	37884	2.53%	0.357%
29	14.433	2096	2099	2103	rVB2	25537	25969	1.73%	0.245%
30	14.480	2103	2107	2114	rBV6	22377	40202	2.68%	0.379%
31	14.810	2160	2163	2168	rVB	23577	29231	1.95%	0.276%
32	15.080	2206	2209	2213	rVB	30022	35631	2.38%	0.336%
33	15.445	2266	2271	2282	rVB	291455	408585	27.25%	3.856%
34	15.674	2307	2310	2317	rVB6	17105	25623	1.71%	0.242%
35	15.915	2347	2351	2355	rBV2	28580	37540	2.50%	0.354%
36	16.739	2486	2491	2496	rVB8	15003	30089	2.01%	0.284%

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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-BF122023.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	17.045	2540	2543	2549	rVB8	13210	22772	1.52%	0.215%
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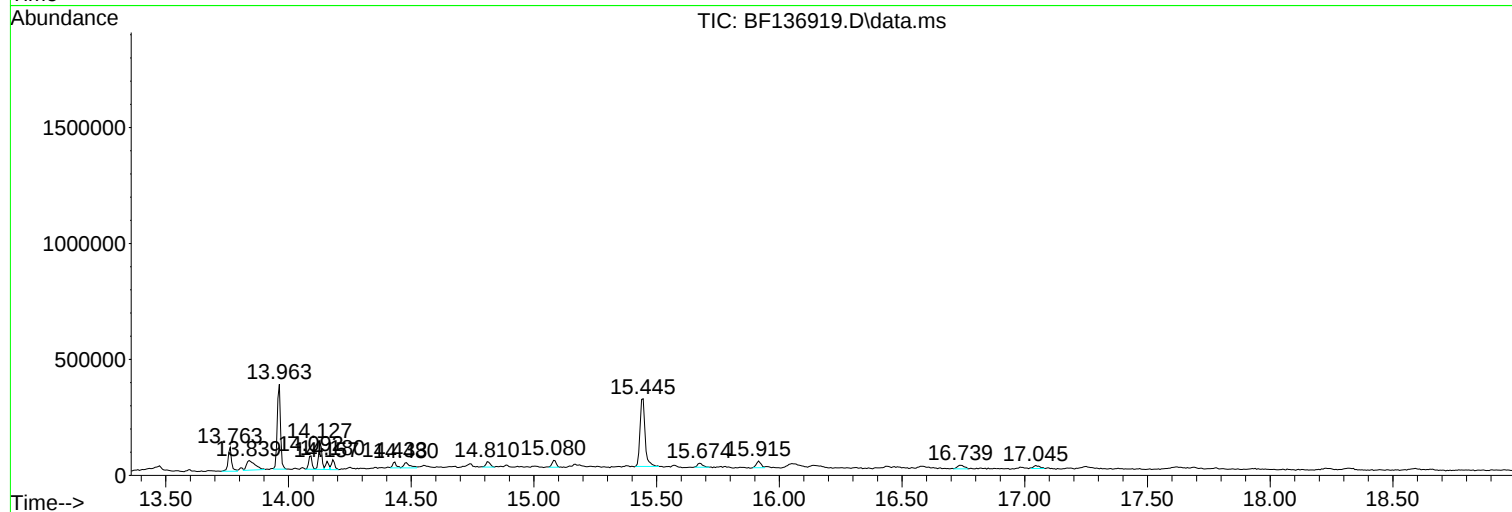
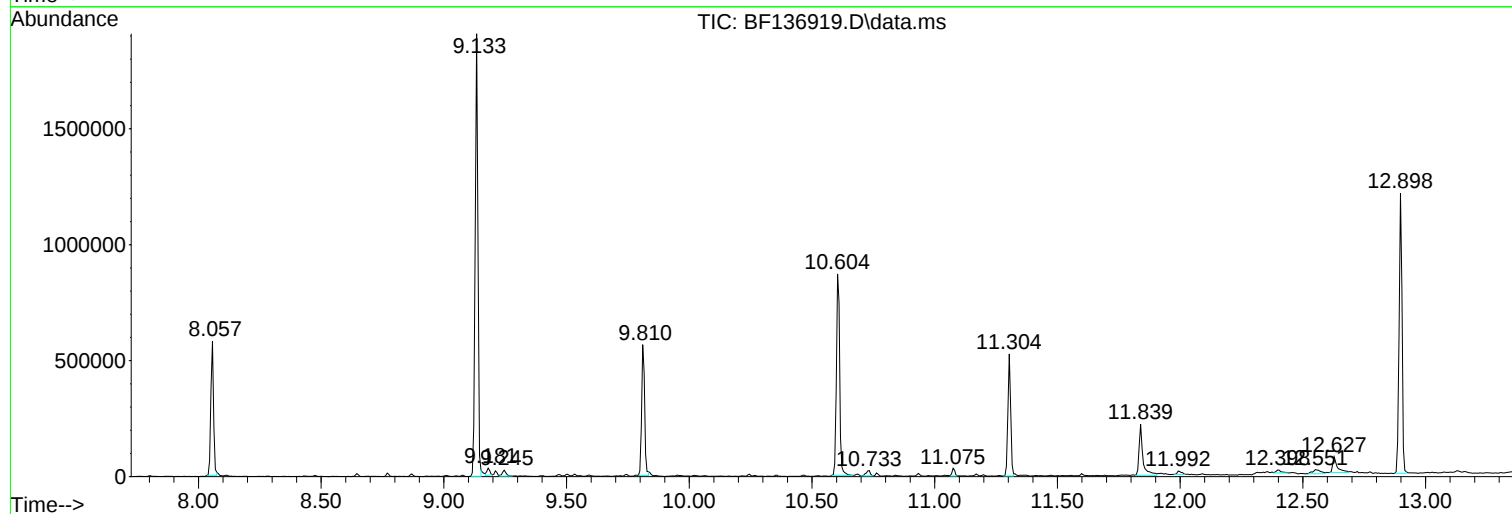
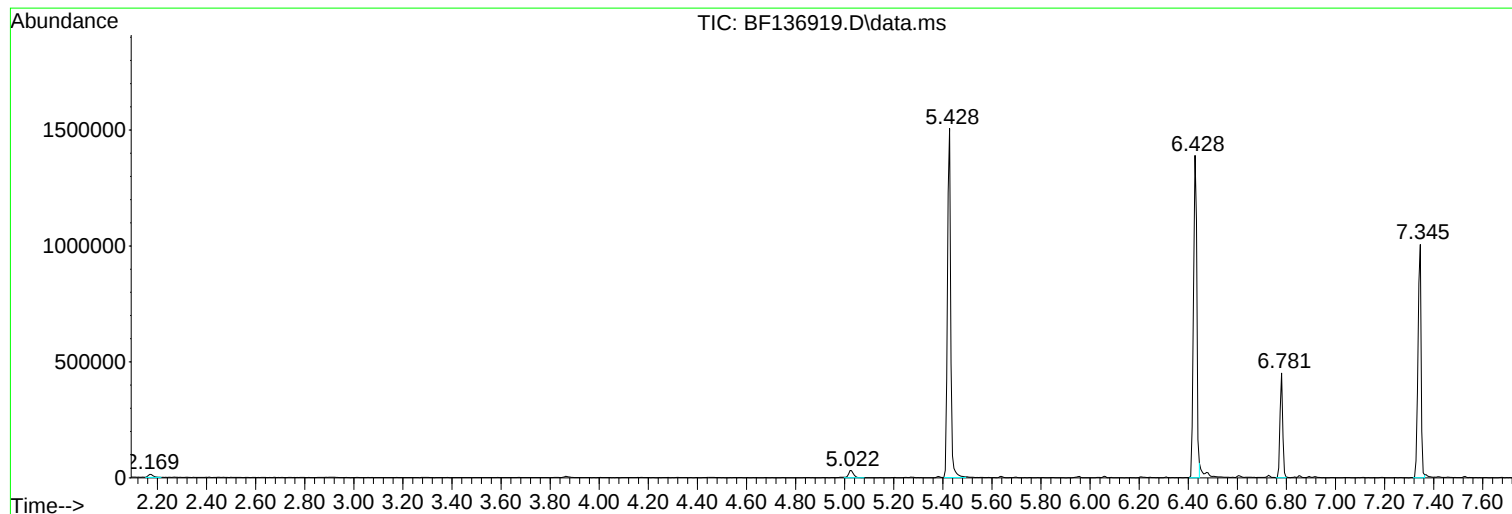
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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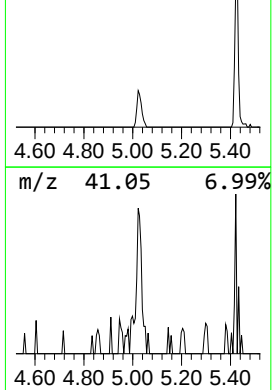
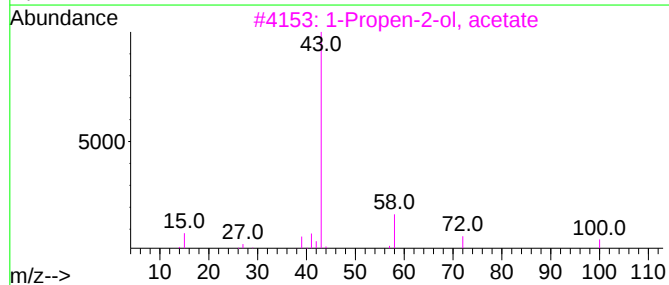
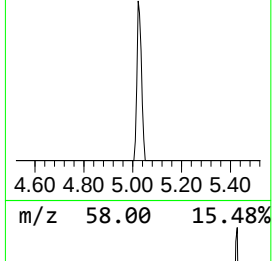
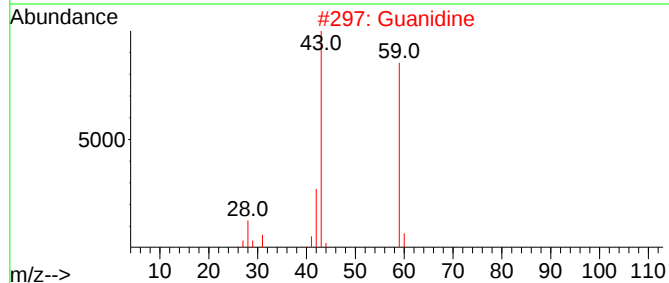
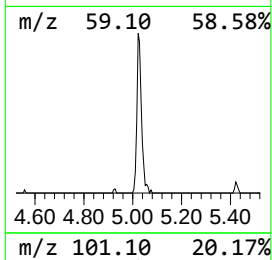
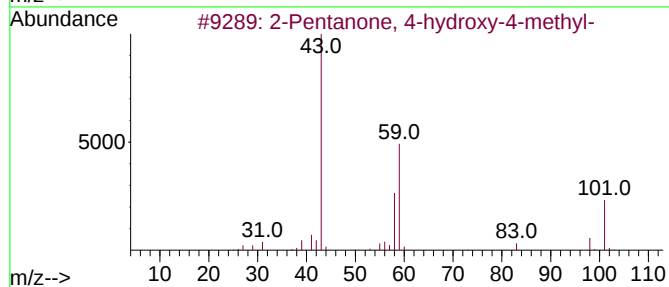
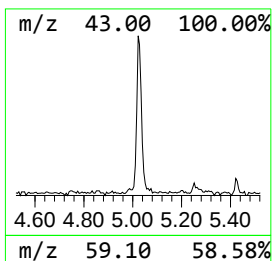
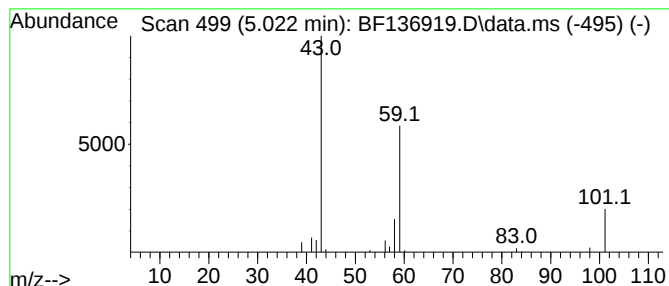
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.M
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TIC Library : C:\Database\NIST20.L
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Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.022	2.60 ng	44981	1,4-Dichlorobenzene-d4	6.781

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50		
2	Guanidine	59	CH5N3	000113-00-8	9		
3	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	9		
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	7		
5	Acetone	58	C3H6O	000067-64-1	5		



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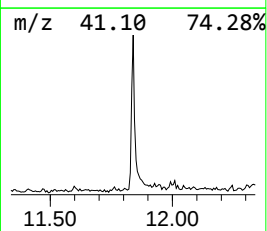
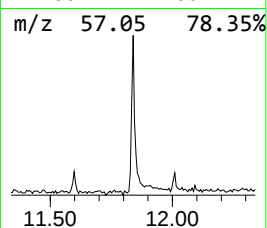
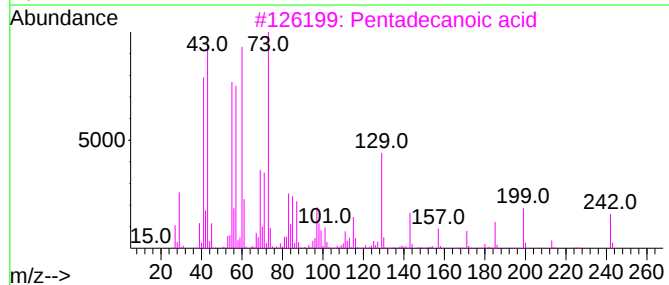
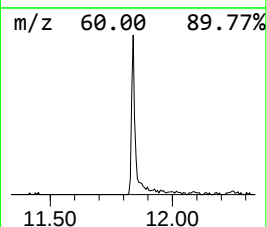
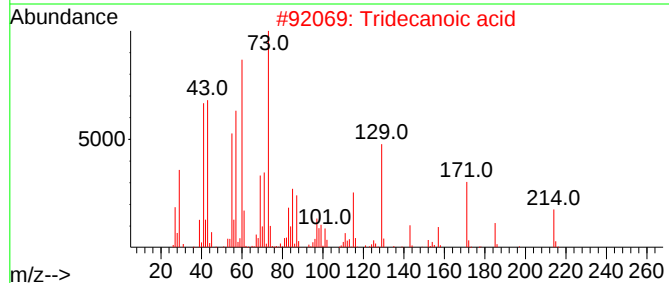
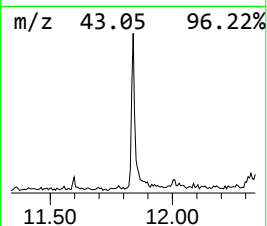
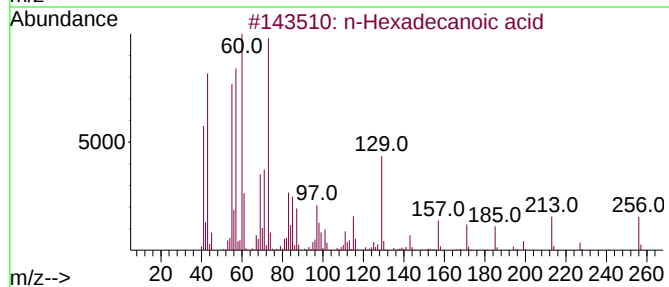
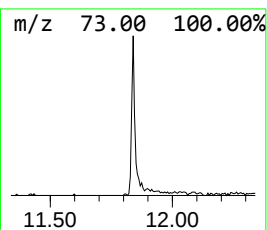
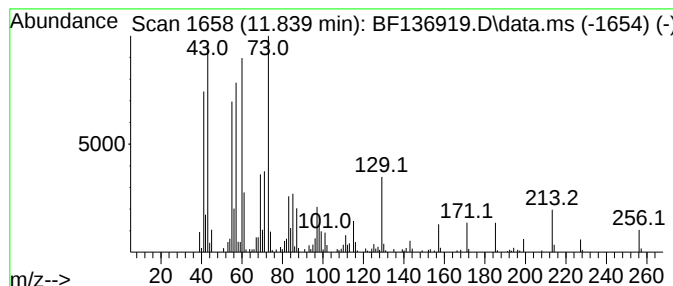
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.839	11.36 ng	235821	Phenanthrene-d10	11.304

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	93
3		Pentadecanoic acid	242	C15H30O2	001002-84-2	72
4		Tetradecanoic acid	228	C14H28O2	000544-63-8	68
5		8-Methylnonanoic acid	172	C10H20O2	005963-14-4	55



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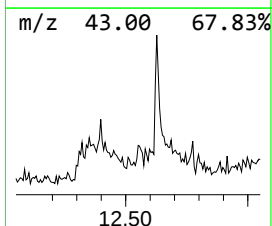
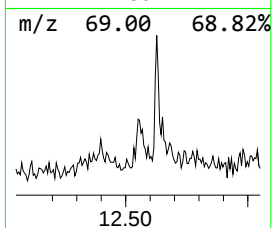
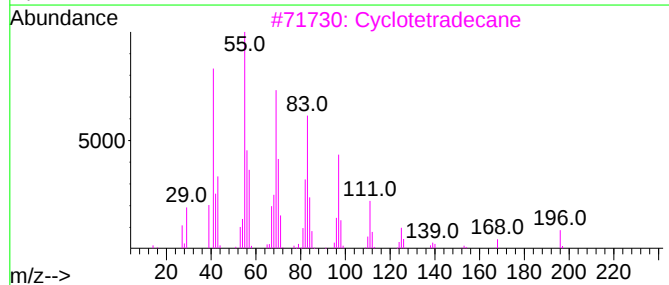
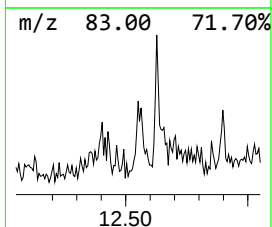
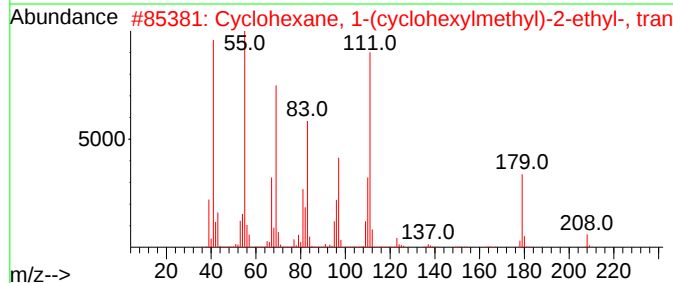
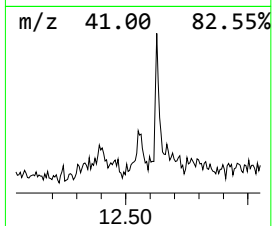
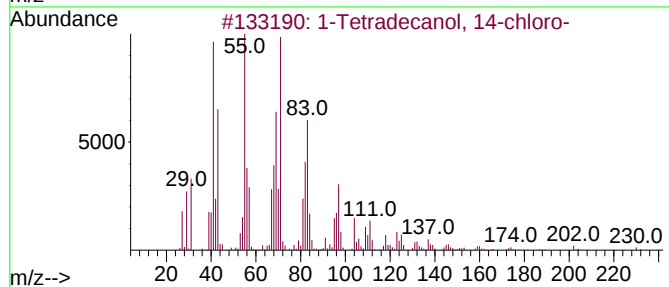
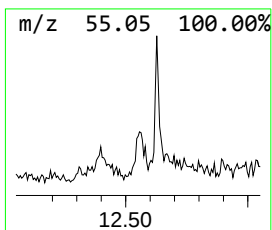
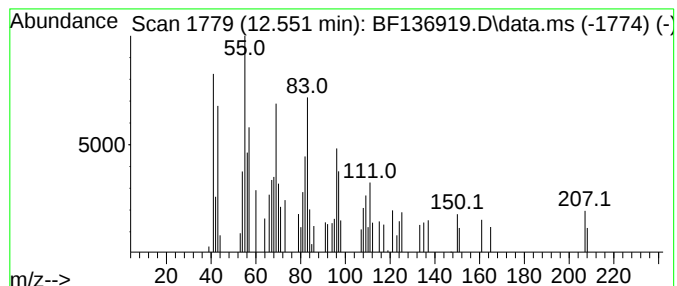
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown12.551 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.551	2.06 ng	42714	Phenanthrene-d10	11.304

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Tetradecanol, 14-chloro-	248	C14H29ClO	073937-05-0	25
2			Cyclohexane, 1-(cyclohexylmethyl)-	208	C15H28	054934-92-8	25
3			Cyclotetradecane	196	C14H28	000295-17-0	22
4			Cyclohexane, 1-(cyclohexylmethyl)-	208	C15H28	054934-94-0	18
5			5-Tetradecanol acetate	256	C16H32O2	051354-25-7	18



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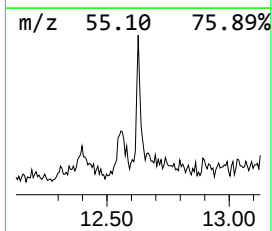
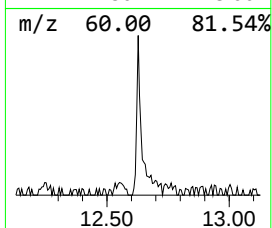
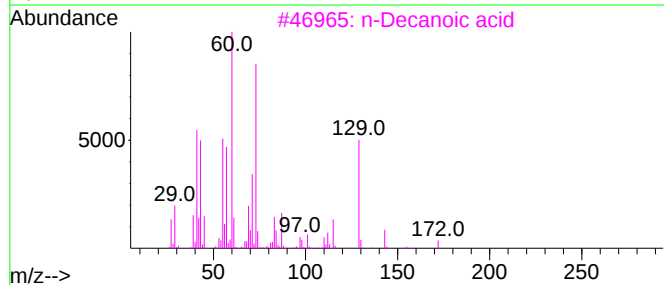
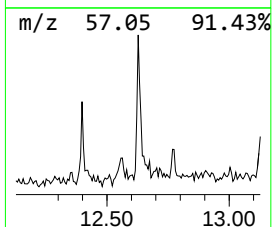
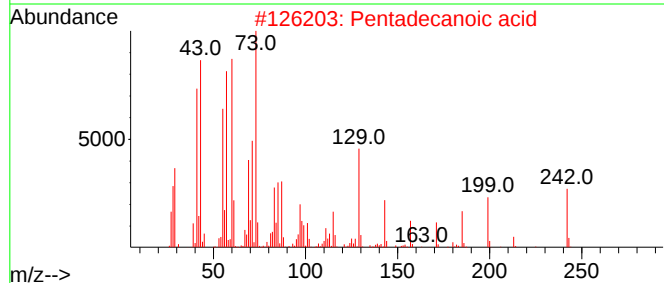
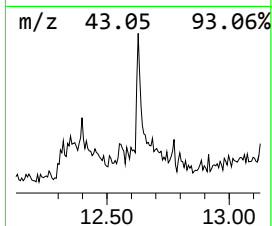
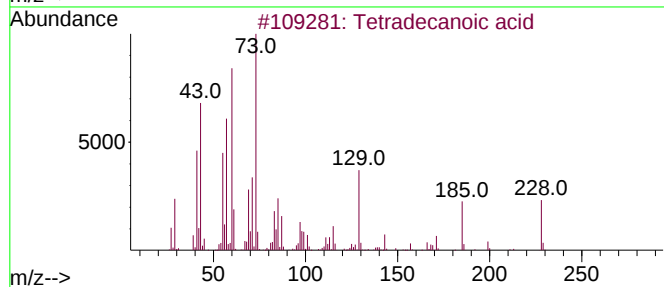
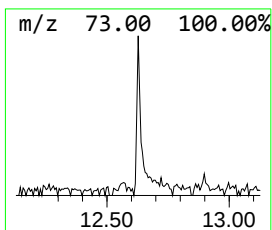
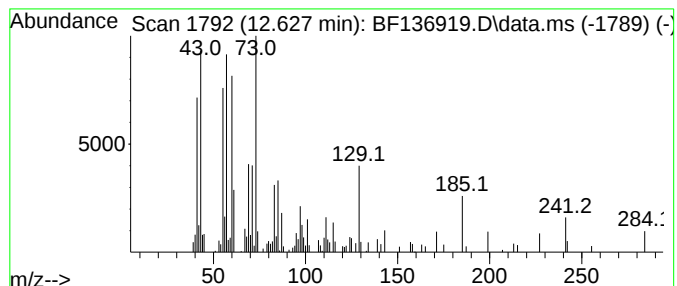
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Tetradecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.627	4.36 ng	90629	Phenanthrene-d10	11.304

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Tetradecanoic acid	228	C14H28O2	000544-63-8	80
2		Pentadecanoic acid	242	C15H30O2	001002-84-2	74
3		n-Decanoic acid	172	C10H20O2	000334-48-5	58
4		Octadecanoic acid	284	C18H36O2	000057-11-4	49
5		Ethanone, 1-(4,5-dihydro-2-thiaz...	129	C5H7NO5	029926-41-8	30



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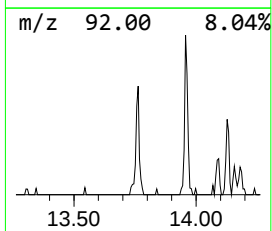
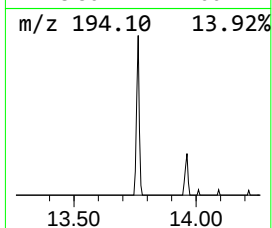
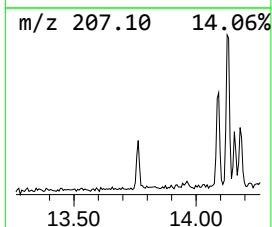
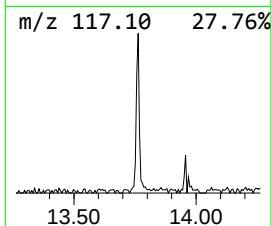
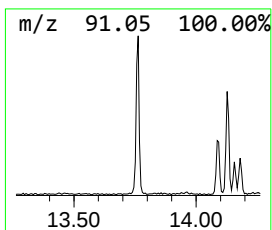
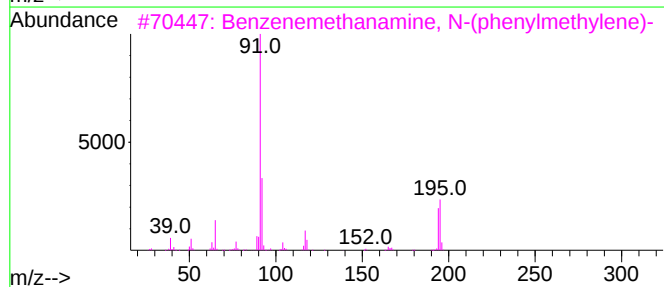
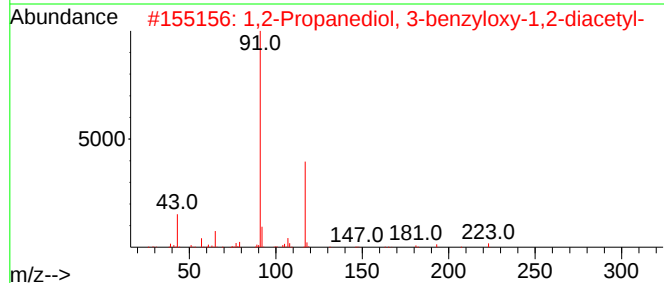
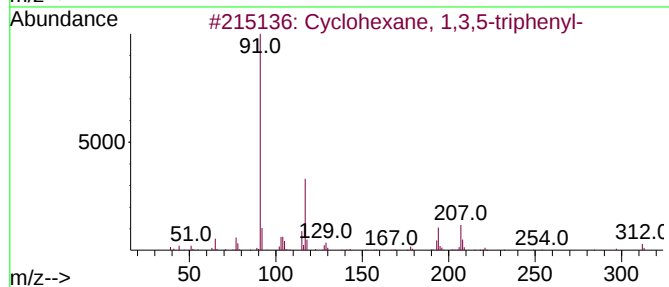
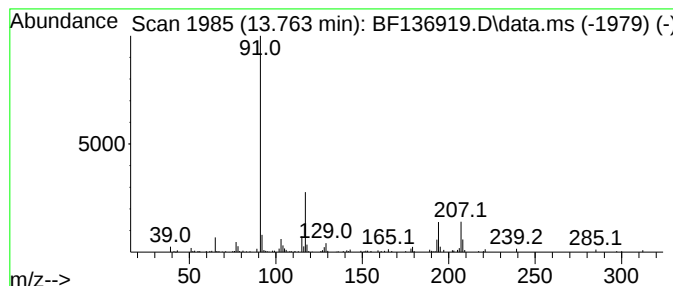
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Cyclohexane, 1,3,5-triphenyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD		R.T.	
13.763	5.93 ng	100910	Chrysene-d12		13.963	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Cyclohexane, 1,3,5-triphenyl-		312	C24H24	028336-57-4	74
2	1,2-Propanediol, 3-benzyloxy-1,2...		266	C14H18O5	013754-10-4	32
3	Benzenemethanamine, N-(phenylmet...		195	C14H13N	000780-25-6	17
4	1-benzylindole		207	C15H13N	1000334-31-3	16
5	Salicylic acid, trimethylsilyl e...		300	C17H20O3Si	1000463-82-7	14



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF010324\
Data File : BF136919.D
Acq On : 03 Jan 2024 21:22
Operator : CG\JU
Sample : 05900-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

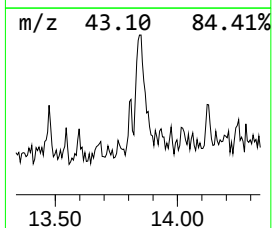
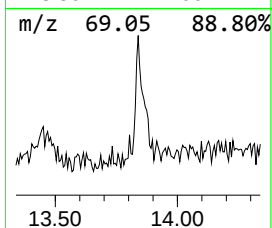
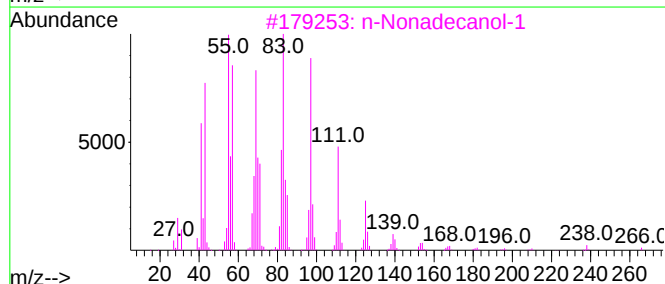
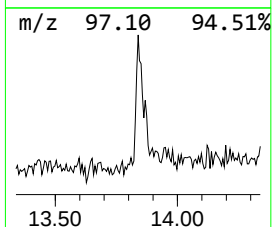
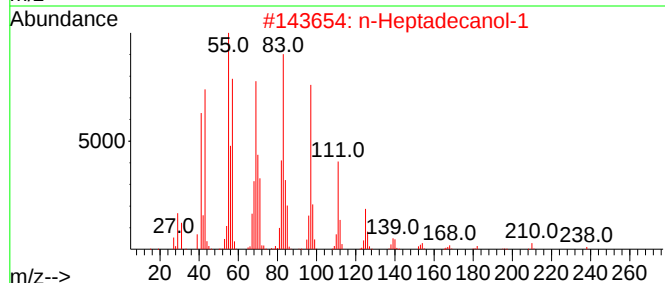
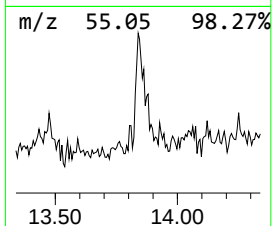
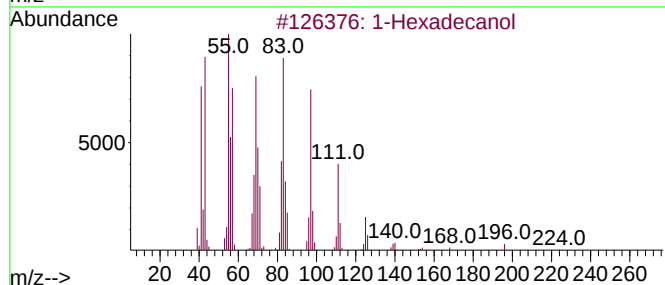
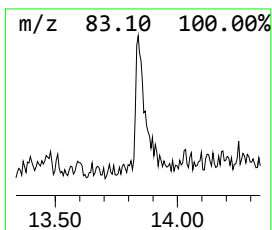
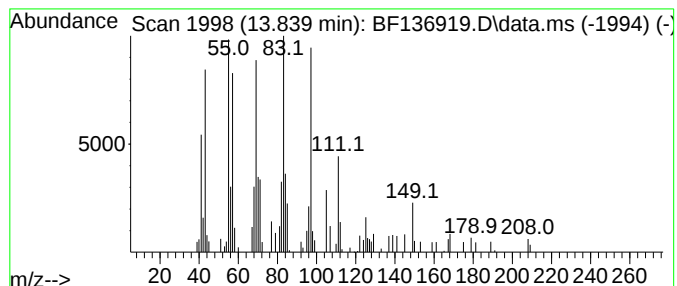
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ClientSampleId :
GHL-SS-54

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 1-Hexadecanol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.839	5.88 ng	99925	Chrysene-d12	13.963	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexadecanol	242	C16H34O	036653-82-4	87
2	n-Heptadecanol-1	256	C17H36O	001454-85-9	72
3	n-Nonadecanol-1	284	C19H40O	001454-84-8	53
4	Cyclopentane, 1,1,3-trimethyl-	112	C8H16	004516-69-2	52
5	Cyclohexane, (1,3-dimethylbutyl)-	168	C12H24	061142-19-6	49



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF010324\
Data File : BF136919.D
Acq On : 03 Jan 2024 21:22
Operator : CG\JU
Sample : 05900-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

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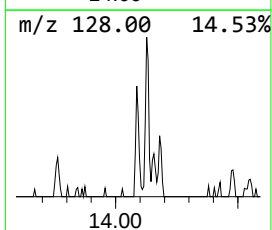
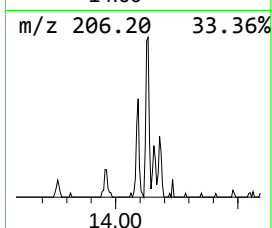
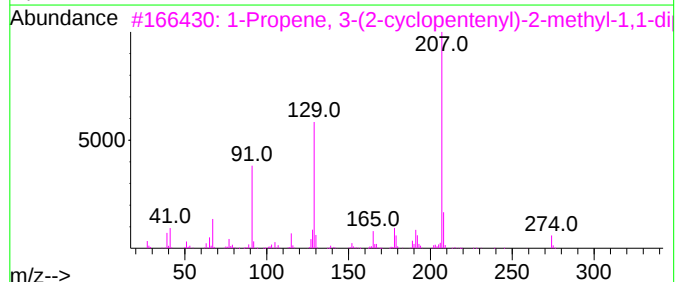
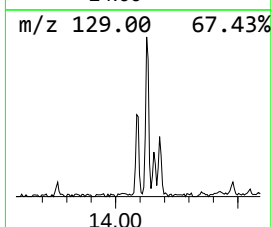
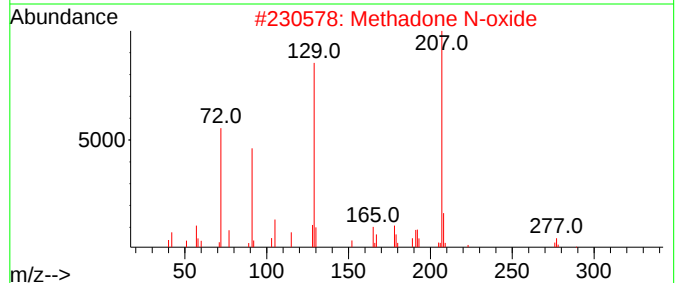
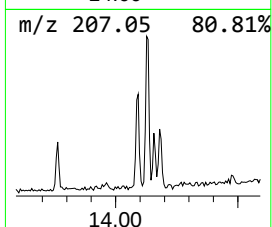
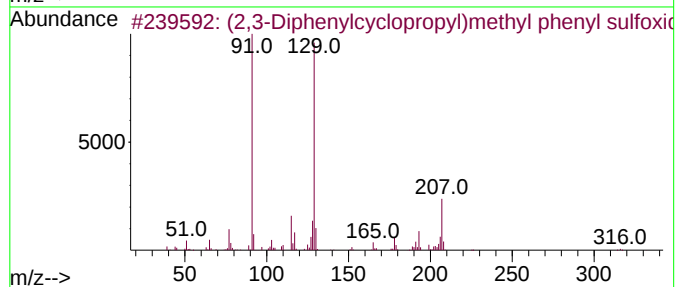
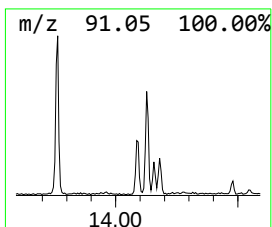
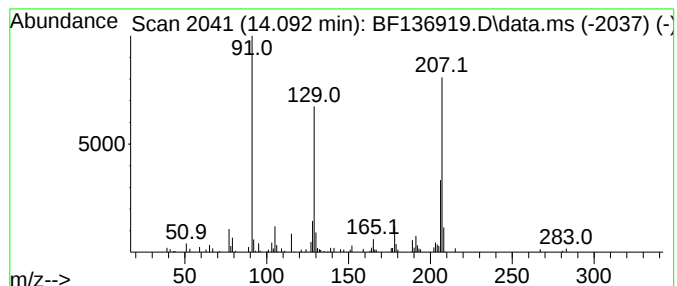
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 (2,3-Diphenylcyclopropyl)me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.092	3.25 ng	55278	Chrysene-d12	13.963

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			(2,3-Diphenylcyclopropyl)methyl ...	332	C22H20OS	131758-71-9	78
2			Methadone N-oxide	325	C21H27NO2	1000120-80-7	64
3			1-Propene, 3-(2-cyclopentenyl)-2...	274	C21H22	1010154-23-3	47
4			5-Methyl-2-phenylindolizine	207	C15H13N	036944-99-7	46
5			Benzo[h]quinoline, 2,4-dimethyl-	207	C15H13N	000605-67-4	46



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF010324\
Data File : BF136919.D
Acq On : 03 Jan 2024 21:22
Operator : CG\JU
Sample : 05900-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

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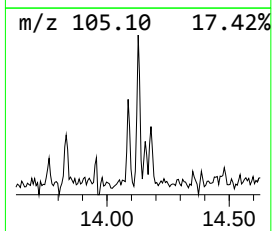
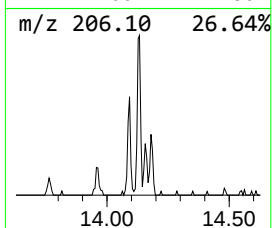
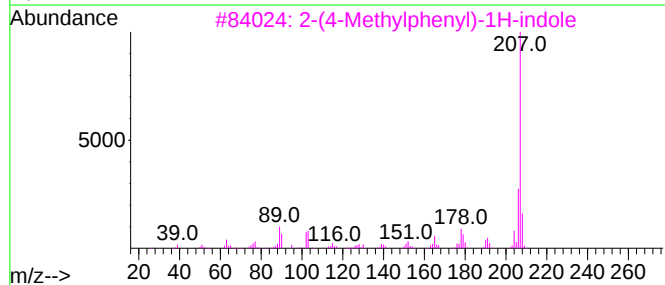
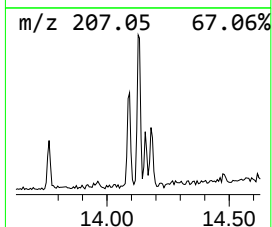
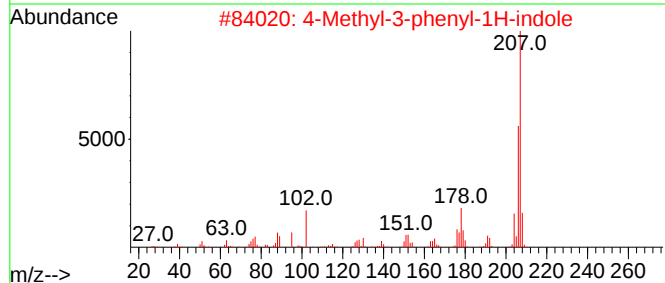
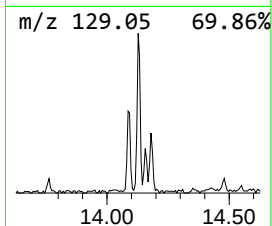
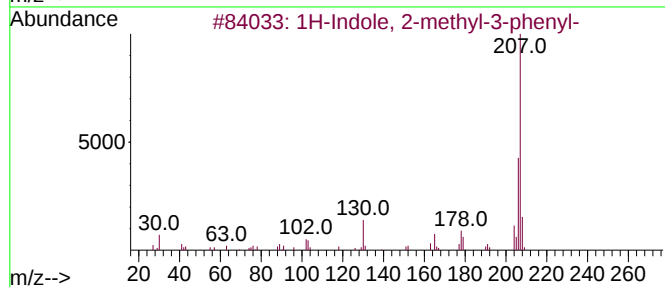
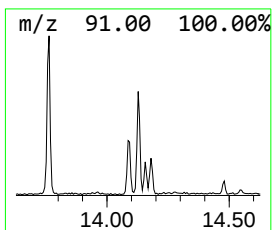
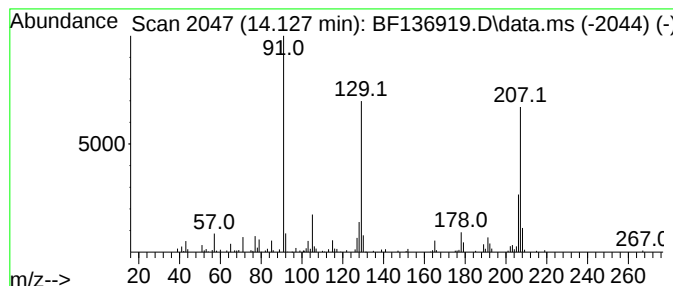
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 1H-Indole, 2-methyl-3-phenyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.127	6.30 ng	107186	Chrysene-d12	13.963

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1H-Indole, 2-methyl-3-phenyl-	207	C15H13N	004757-69-1	50
2			4-Methyl-3-phenyl-1H-indole	207	C15H13N	180271-54-9	43
3			2-(4-Methylphenyl)-1H-indole	207	C15H13N	055577-25-8	38
4			1H-Indole, 1-methyl-2-phenyl-	207	C15H13N	003558-24-5	38
5			5-Methyl-2-phenylindolizine	207	C15H13N	036944-99-7	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF010324\
Data File : BF136919.D
Acq On : 03 Jan 2024 21:22
Operator : CG\JU
Sample : 05900-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

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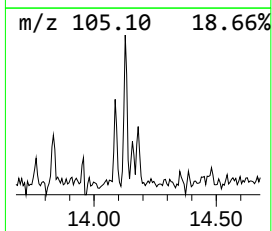
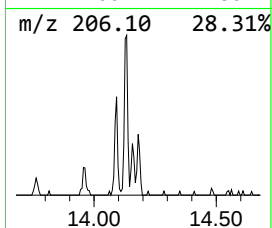
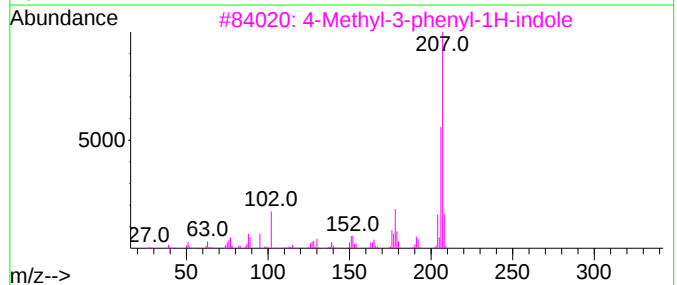
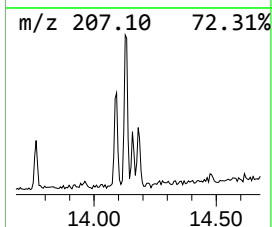
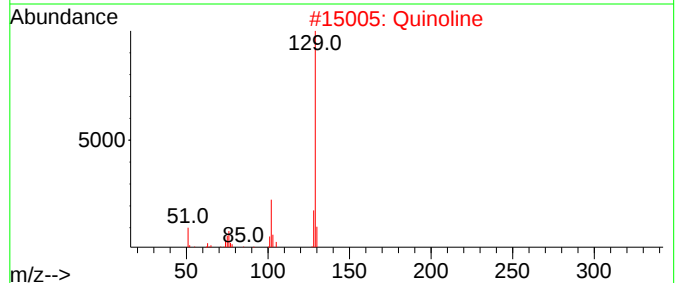
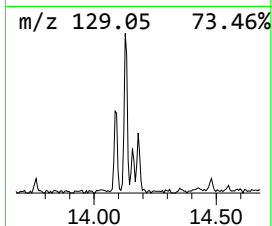
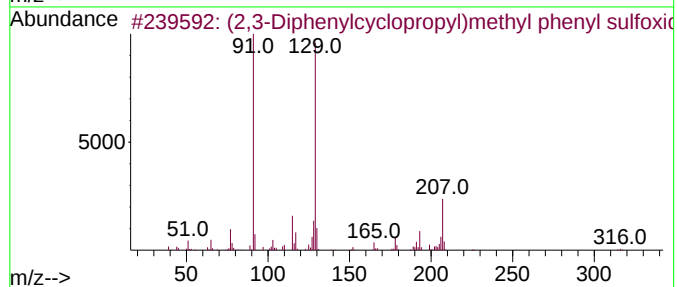
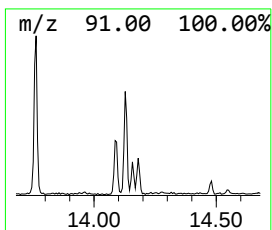
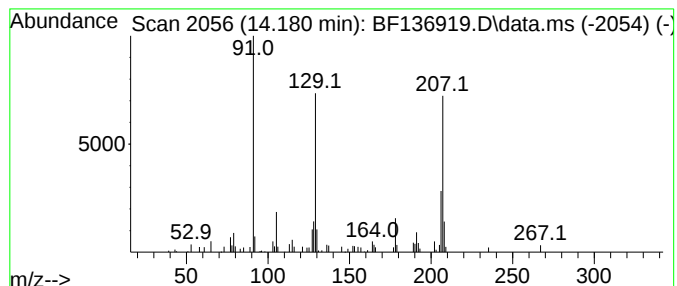
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 unknown14.180 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.180	2.23 ng	37884	Chrysene-d12	13.963

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			(2,3-Diphenylcyclopropyl)methyl ...	332	C22H20O5	131758-71-9	50
2			Quinoline	129	C9H7N	000091-22-5	38
3			4-Methyl-3-phenyl-1H-indole	207	C15H13N	180271-54-9	35
4			5-Methyl-2-phenylindolizine	207	C15H13N	036944-99-7	30
5			1H-Indole, 1-methyl-2-phenyl-	207	C15H13N	003558-24-5	30



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF010324\
Data File : BF136919.D
Acq On : 03 Jan 2024 21:22
Operator : CG\JU
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Misc :
ALS Vial : 10 Sample Multiplier: 1

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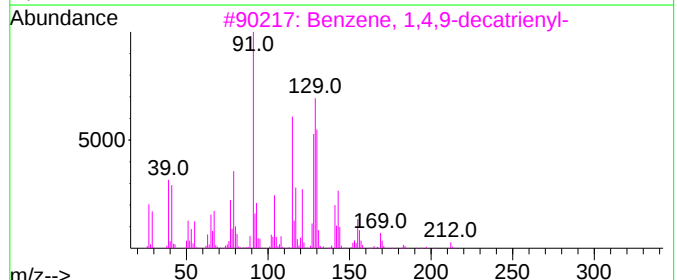
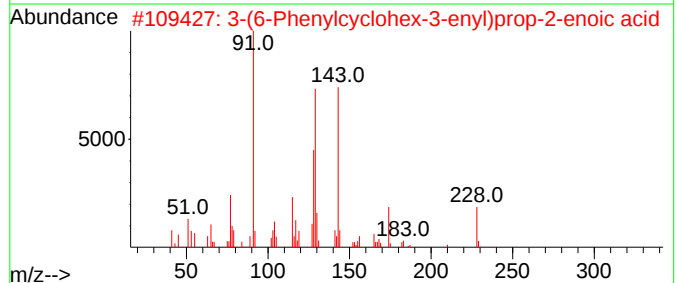
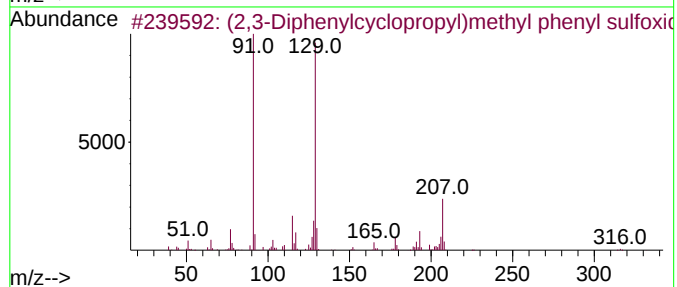
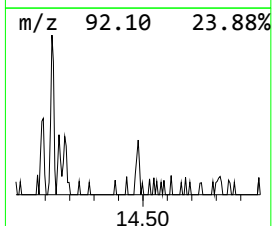
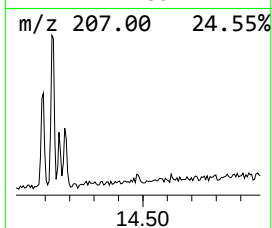
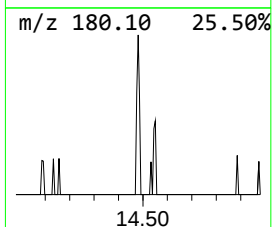
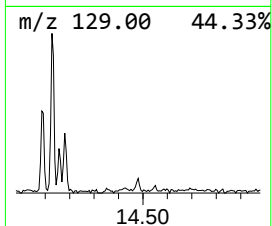
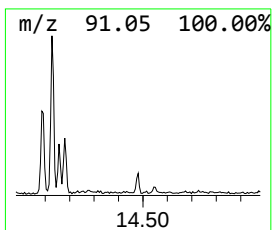
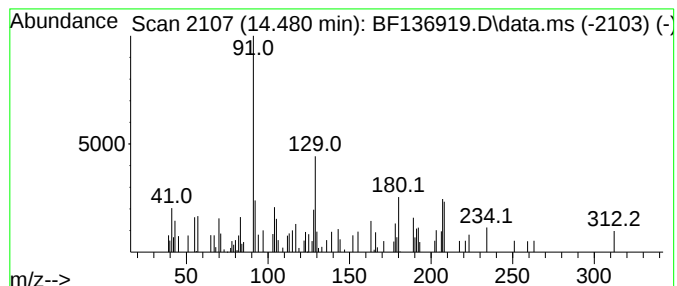
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 unknown14.480 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.480	2.36 ng	40202	Chrysene-d12	13.963

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			(2,3-Diphenylcyclopropyl)methyl ...	332	C22H20O5	131758-71-9	25
2			3-(6-Phenylcyclohex-3-enyl)prop-...	228	C15H16O2	1000215-26-7	10
3			Benzene, 1,4,9-decatrienyl-	212	C16H20	013393-63-0	10
4			Cyclohexane, 1,3,5-triphenyl-	312	C24H24	028336-57-4	9
5			1-Ethyl-3,3-bis(trifluoromethyl)...	208	C5H6F6N2	032770-47-1	9



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF010324\
Data File : BF136919.D
Acq On : 03 Jan 2024 21:22
Operator : CG\JU
Sample : 05900-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.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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n-Hexadecanoic ...	11.839	11.4	ng	235821	4	11.304	415326	20.0
unknown12.551	12.551	2.1	ng	42714	4	11.304	415326	20.0
Tetradecanoic acid	12.627	4.4	ng	90629	4	11.304	415326	20.0
Cyclohexane, 1,...	13.763	5.9	ng	100910	5	13.963	340072	20.0
1-Hexadecanol	13.839	5.9	ng	99925	5	13.963	340072	20.0
(2,3-Diphenylcy...	14.092	3.3	ng	55278	5	13.963	340072	20.0
1H-Indole, 2-me...	14.127	6.3	ng	107186	5	13.963	340072	20.0
unknown14.180	14.180	2.2	ng	37884	5	13.963	340072	20.0
unknown14.480	14.480	2.4	ng	40202	5	13.963	340072	20.0