

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080223\
 Data File : BF134592.D
 Acq On : 02 Aug 2023 21:45
 Operator : CG\JU
 Sample : 03834-02
 Misc :
 ALS Vial : 23 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 B-P2B

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-BF080123.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF134592.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.016	495	498	507	rVB	35301	39457	1.68%	0.194%
2	5.416	561	566	569	rBV	2477759	2128071	90.66%	10.442%
3	6.422	732	737	740	rBV	2449206	2204817	93.93%	10.819%
4	6.622	768	771	776	rBV	60460	49340	2.10%	0.242%
5	6.792	797	800	804	rBV	1273432	1026162	43.72%	5.035%
6	7.351	891	895	898	rBV	1643927	1290094	54.96%	6.330%
7	8.069	1014	1017	1021	rVB	1479208	1287017	54.83%	6.315%
8	9.151	1197	1201	1204	rVB	2695423	2257121	96.16%	11.076%
9	9.269	1218	1221	1225	rBV	58271	45821	1.95%	0.225%
10	9.828	1312	1316	1319	rBV	1407001	1171866	49.93%	5.750%
11	10.610	1445	1449	1453	rBV	1384666	1168152	49.77%	5.732%
12	10.657	1454	1457	1460	rVB	40010	33276	1.42%	0.163%
13	11.310	1565	1568	1572	rBV	1171649	1050752	44.77%	5.156%
14	11.851	1656	1660	1665	rBV	189567	185939	7.92%	0.912%
15	12.521	1771	1774	1778	rBV	31999	36431	1.55%	0.179%
16	12.639	1791	1794	1800	rBV	44668	49480	2.11%	0.243%
17	12.904	1836	1839	1843	rVB	2105961	1885956	80.35%	9.254%
18	13.821	1991	1995	2002	rVB	184522	196345	8.37%	0.963%
19	13.957	2014	2018	2022	rBV	2764731	2347199	100.00%	11.518%
20	14.145	2047	2050	2056	rVB	28533	33631	1.43%	0.165%
21	14.451	2099	2102	2110	rVB3	48908	74001	3.15%	0.363%
22	14.757	2151	2154	2159	rVB3	27102	32877	1.40%	0.161%
23	14.833	2163	2167	2173	rBV	197790	192977	8.22%	0.947%
24	14.904	2177	2179	2183	rVB3	35360	36081	1.54%	0.177%
25	15.104	2210	2213	2216	rBV	84588	85679	3.65%	0.420%
26	15.133	2216	2218	2225	rVB6	29653	36655	1.56%	0.180%
27	15.421	2262	2267	2275	rBV	489423	624803	26.62%	3.066%
28	15.698	2310	2314	2319	rVB2	54453	72342	3.08%	0.355%
29	15.939	2352	2355	2360	rVB2	49390	65480	2.79%	0.321%
30	15.998	2361	2365	2371	rVB2	44210	77383	3.30%	0.380%
31	16.333	2419	2422	2429	rVB8	32270	59772	2.55%	0.293%
32	16.762	2490	2495	2504	rVB3	86584	171511	7.31%	0.842%
33	17.092	2549	2551	2558	rVB8	39299	68566	2.92%	0.336%
34	17.180	2562	2566	2571	rBV6	23394	45449	1.94%	0.223%
35	17.539	2622	2627	2638	rVB6	60331	150711	6.42%	0.740%
36	18.580	2799	2804	2816	rVB10	37884	97917	4.17%	0.480%

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Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

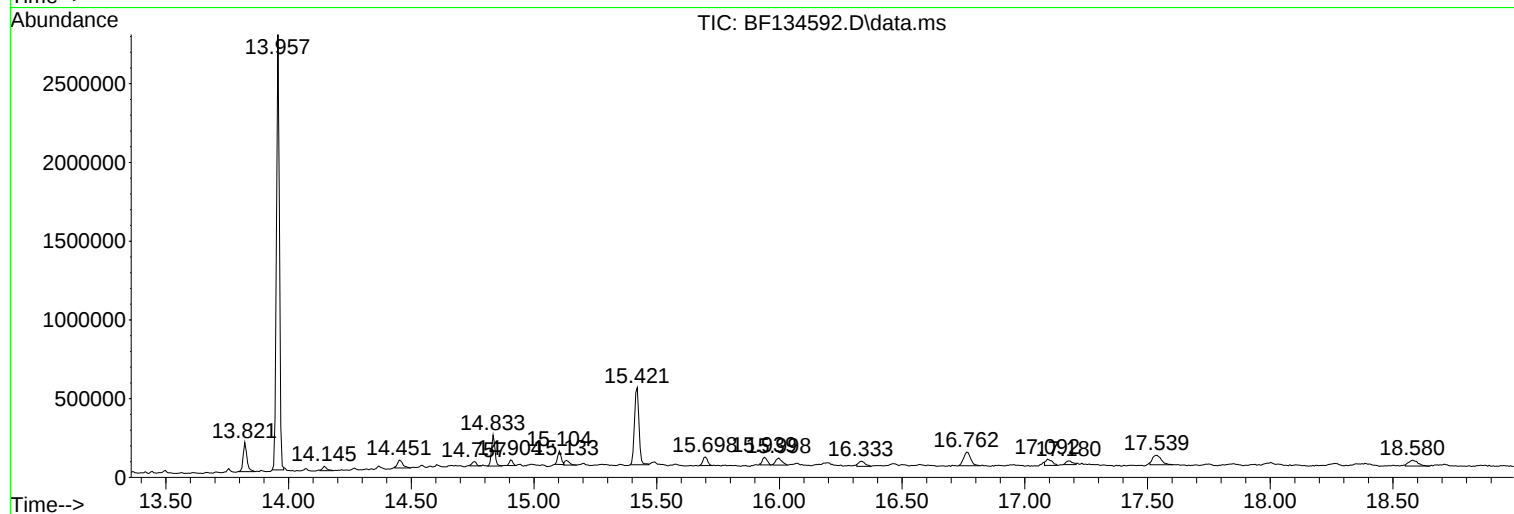
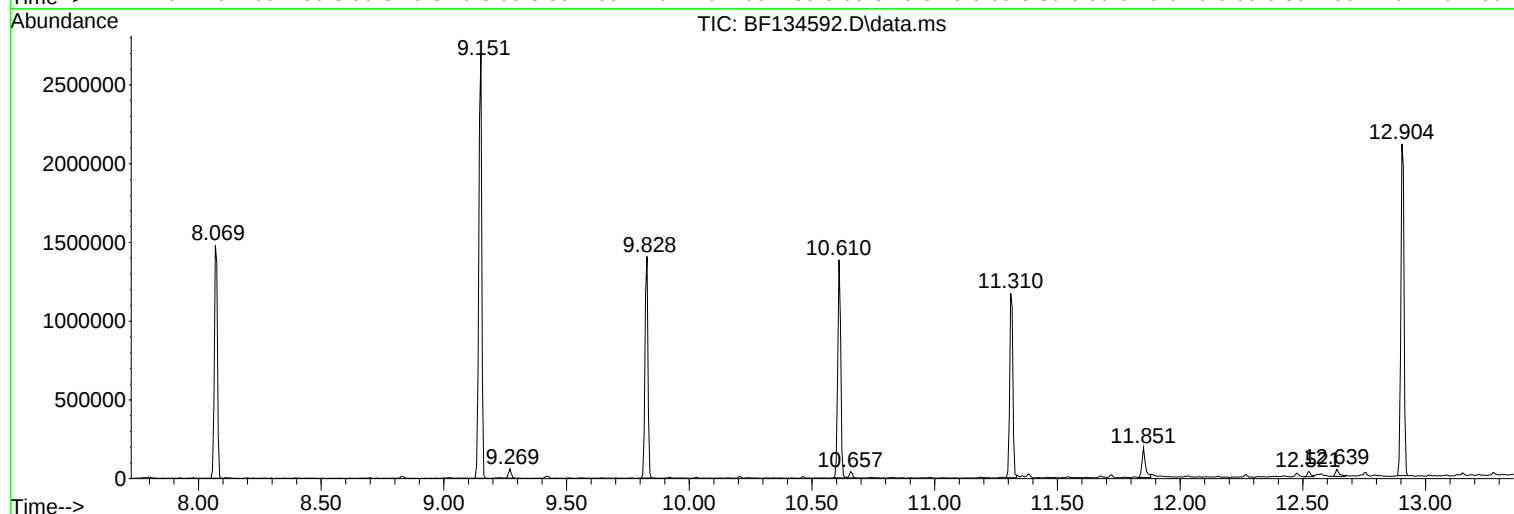
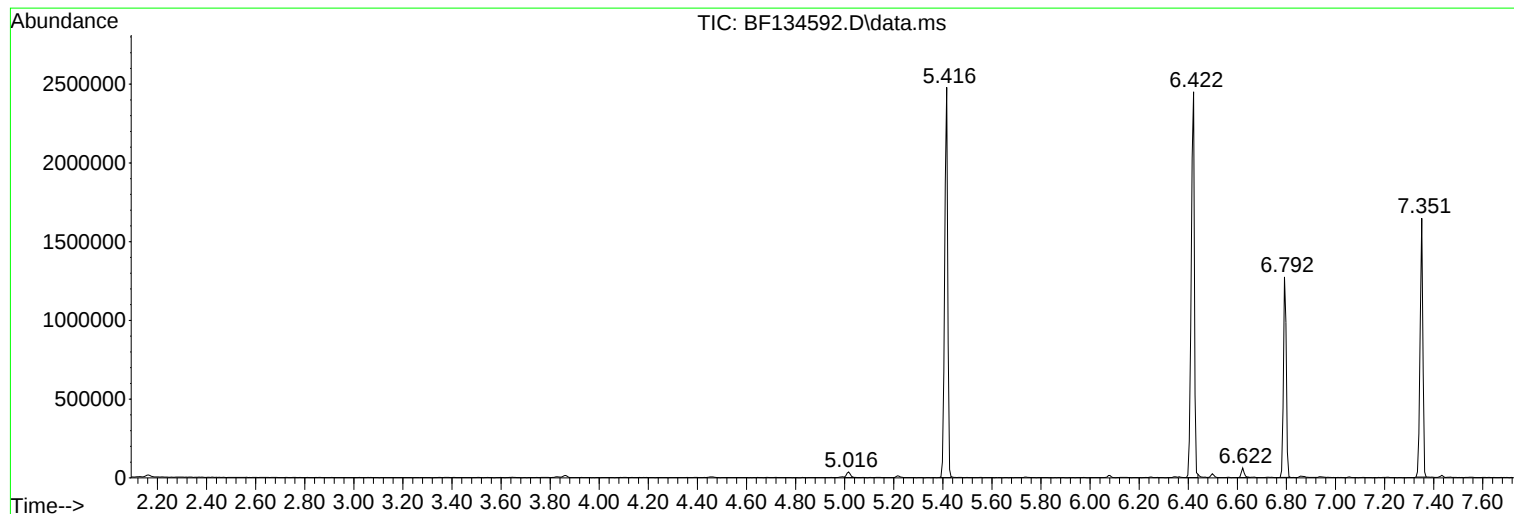
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF080123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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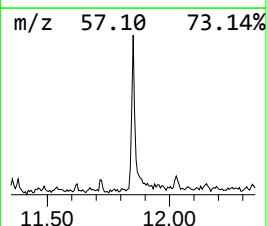
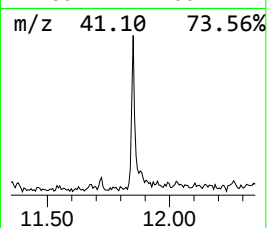
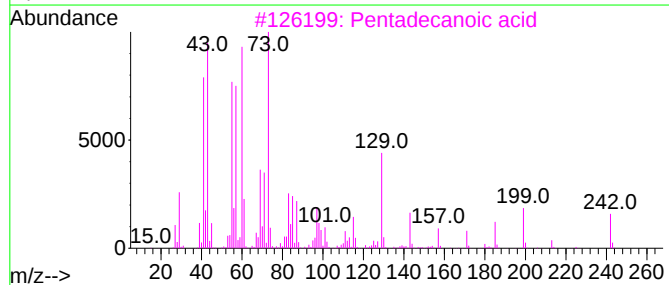
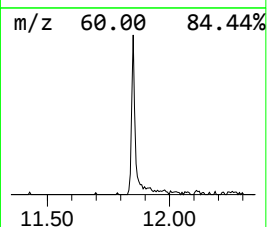
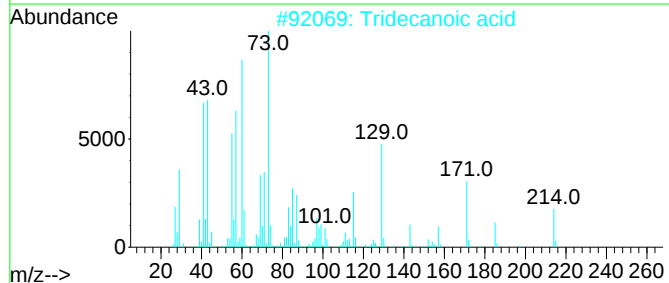
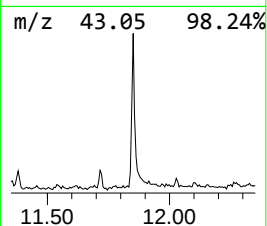
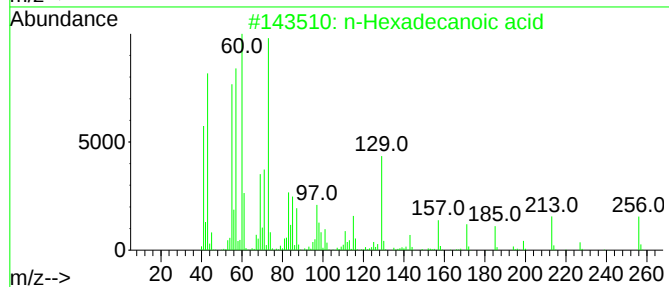
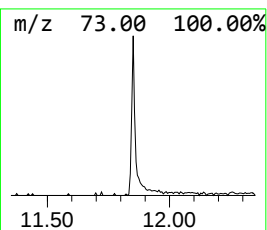
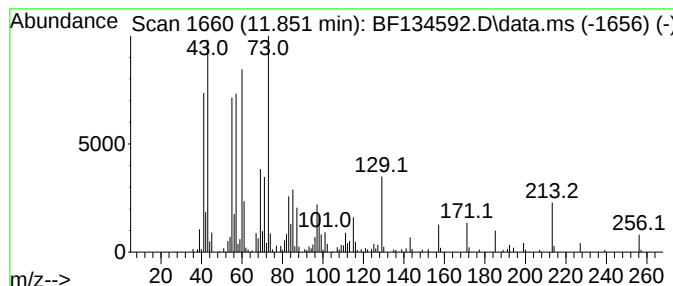
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF080123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.851	3.54 ng	185939	Phenanthrene-d10	11.310

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	95
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	87
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	72
5			Dodecanoic acid	200	C12H24O2	000143-07-7	64



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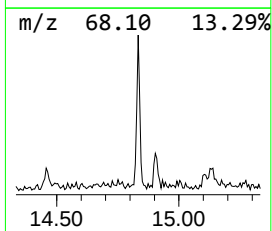
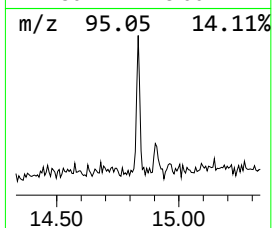
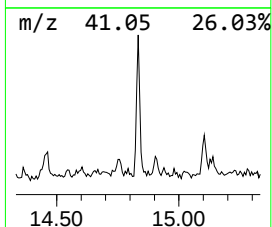
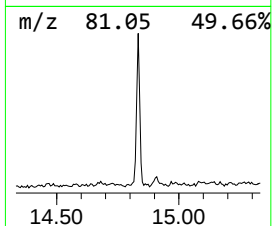
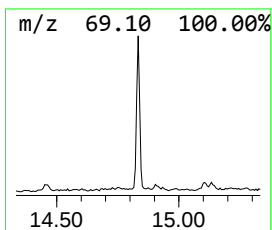
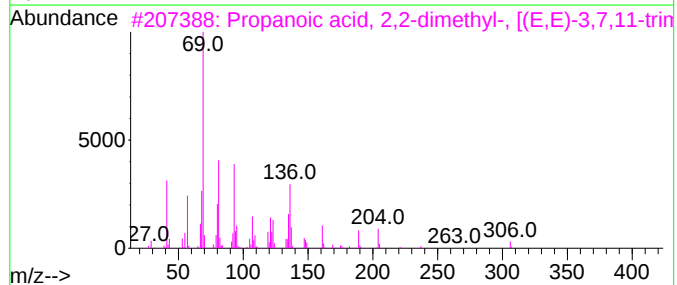
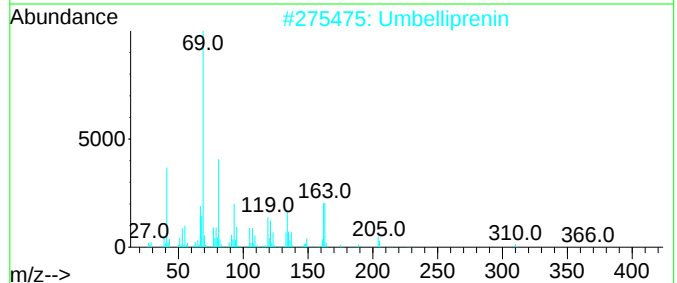
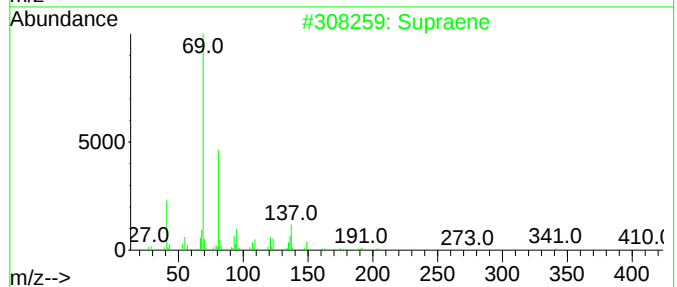
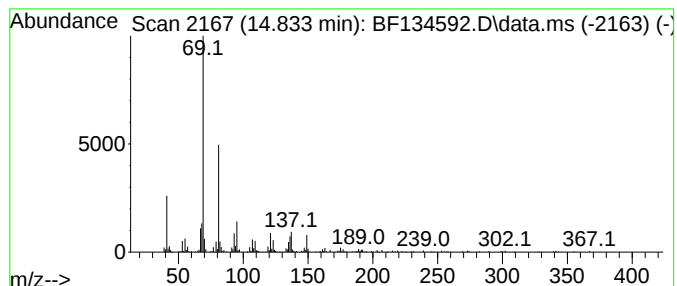
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Peak Number 2 Supraene Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.833	6.18 ng	192977	Perylene-d12	15.421

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Supraene	410	C30H50	007683-64-9	90
2			Umbelliprenin	366	C24H30O3	023838-17-7	72
3			Propanoic acid, 2,2-dimethyl-, [...	306	C20H34O2	1000164-38-8	64
4			1,5-Heptadiene, 3,3,6-trimethyl-	138	C10H18	035387-63-4	52
5			1,5-Heptadiene, 2,3,6-trimethyl-	138	C10H18	033501-88-1	50



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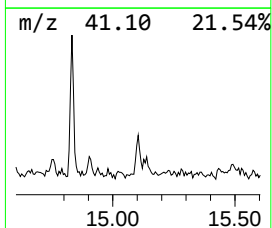
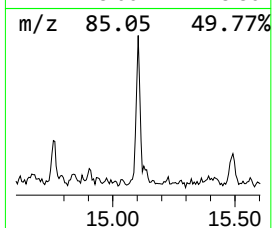
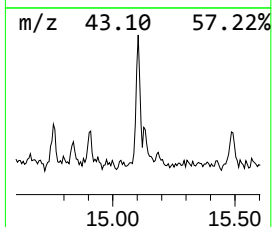
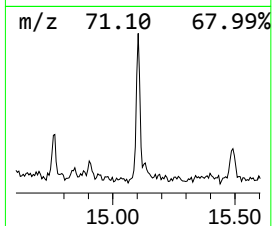
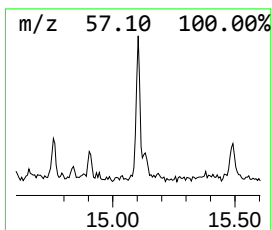
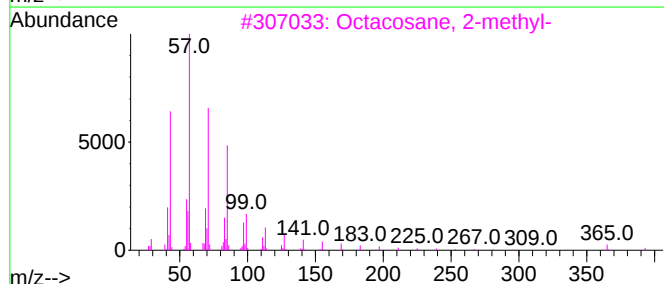
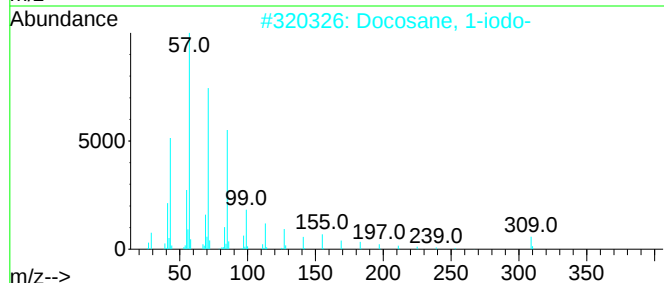
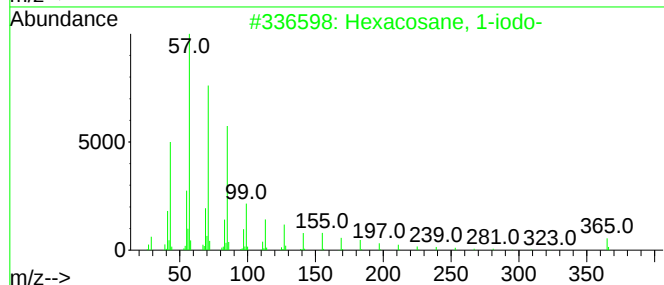
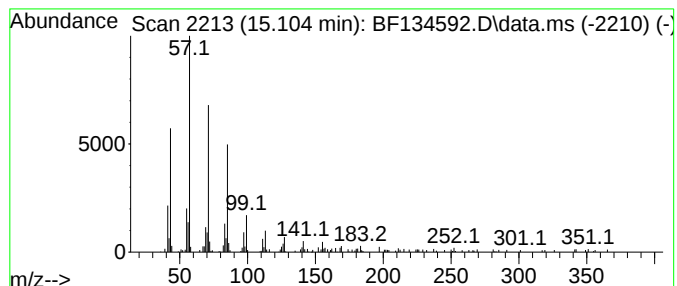
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Hexacosane, 1-iodo- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.104	2.74 ng	85679	Perylene-d12	15.421

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexacosane, 1-iodo-	492	C26H53I	1000406-32-1	91
2			Docosane, 1-iodo-	436	C22H45I	1000406-31-9	90
3			Octacosane, 2-methyl-	408	C29H60	001560-98-1	90
4			Hexacosane	366	C26H54	000630-01-3	87
5			Pentacosane	352	C25H52	000629-99-2	87



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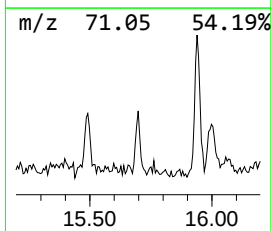
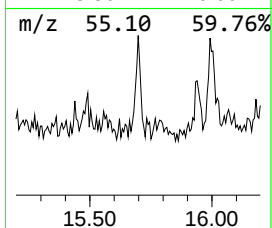
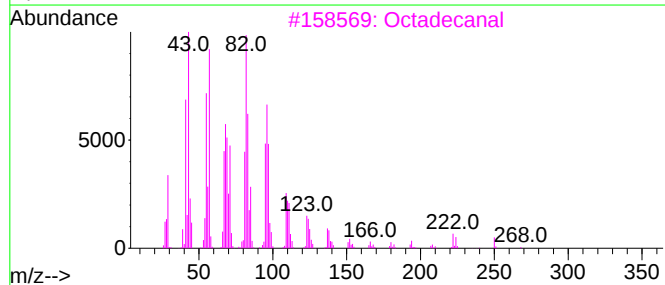
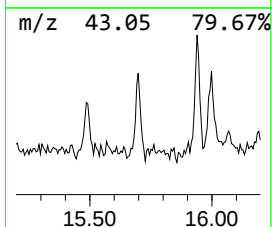
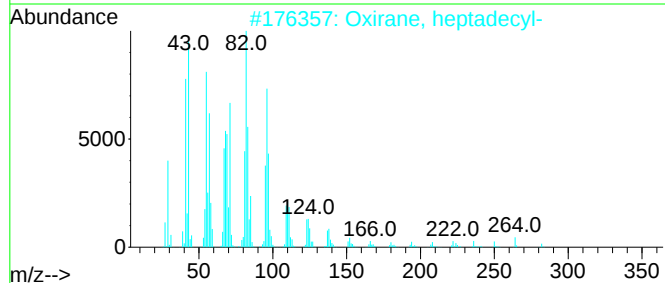
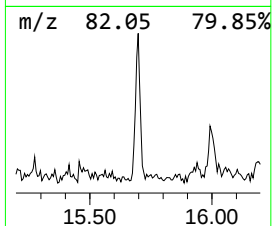
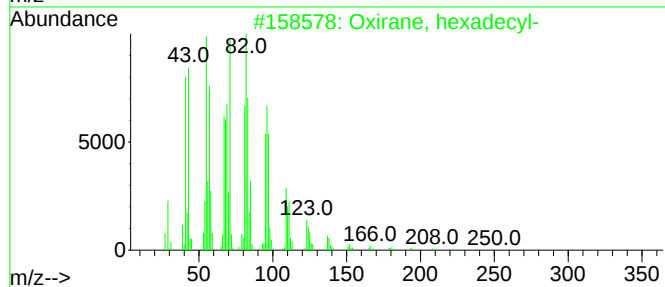
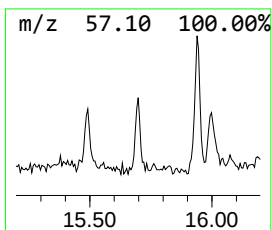
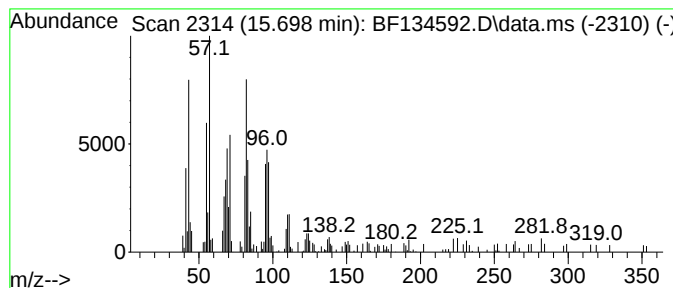
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Peak Number 4 Oxirane, hexadecyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.698	2.32 ng	72342	Perylene-d12	15.421

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Oxirane, hexadecyl-	268	C18H36O	007390-81-0	86
2			Oxirane, heptadecyl-	282	C19H38O	067860-04-2	81
3			Octadecanal	268	C18H36O	000638-66-4	80
4			1,19-Eicosadiene	278	C20H38	014811-95-1	72
5			Tetracosanal	352	C24H48O	057866-08-7	62



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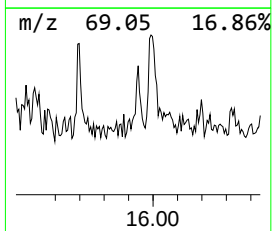
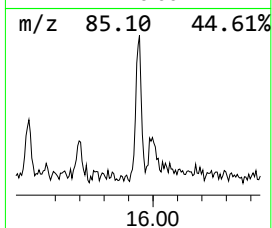
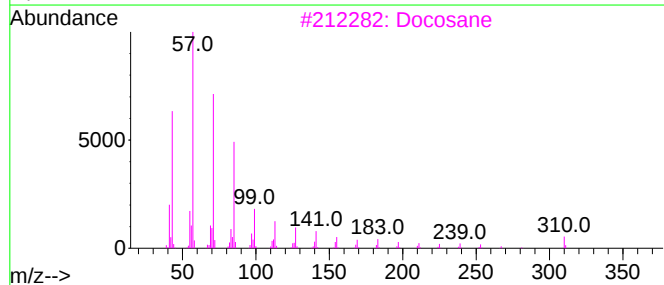
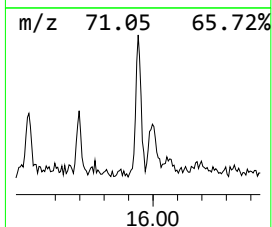
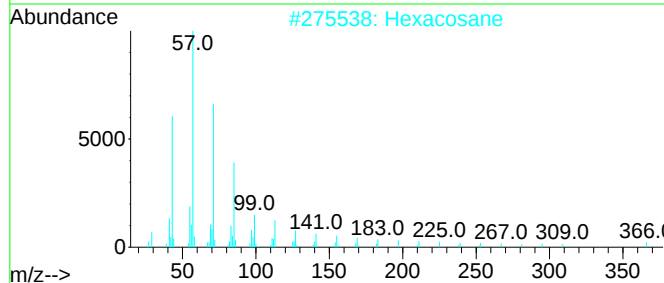
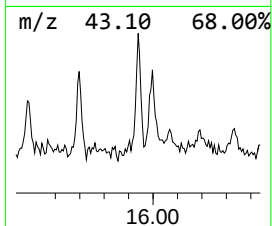
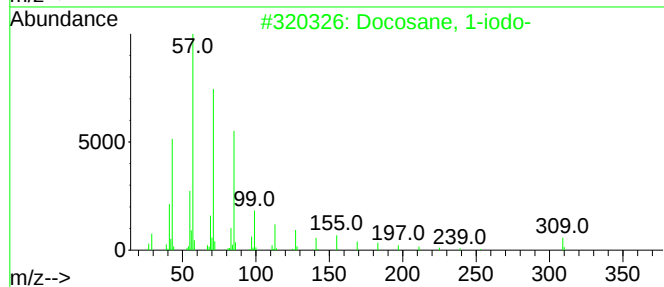
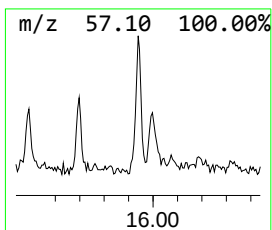
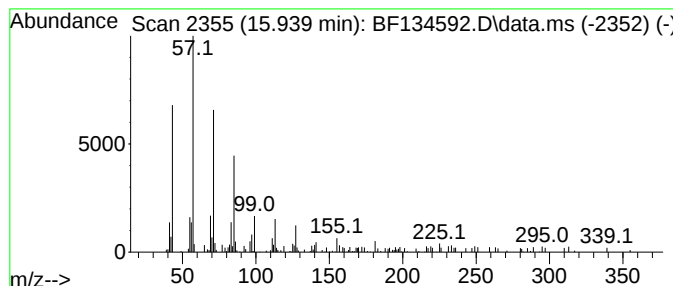
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Peak Number 5 Docosane, 1-iodo- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.939	2.10 ng	65480	Perylene-d12	15.421

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Docosane, 1-iodo-	436	C22H45I	1000406-31-9	91
2			Hexacosane	366	C26H54	000630-01-3	90
3			Docosane	310	C22H46	000629-97-0	90
4			Tetracosane	338	C24H50	000646-31-1	90
5			Octadecane, 1-iodo-	380	C18H37I	000629-93-6	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080223\
Data File : BF134592.D
Acq On : 02 Aug 2023 21:45
Operator : CG\JU
Sample : 03834-02
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
B-P2B

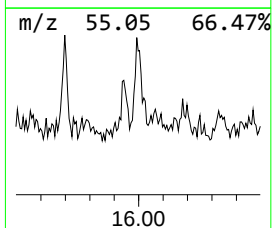
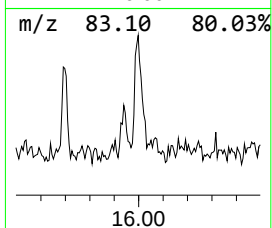
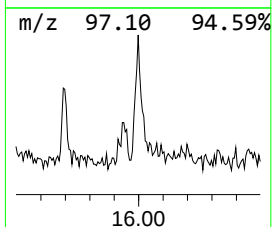
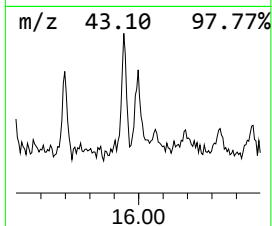
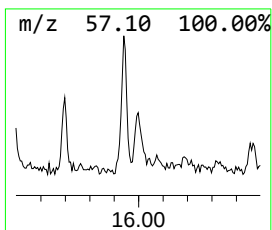
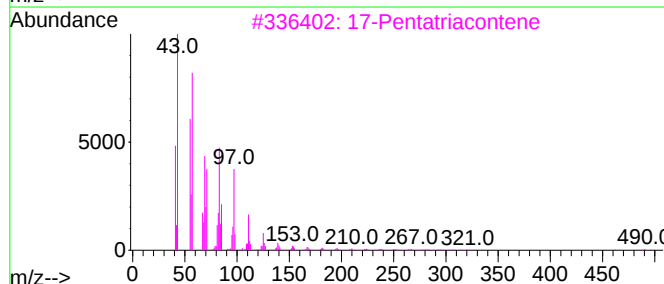
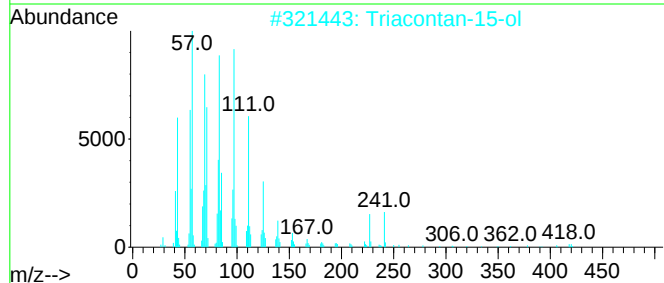
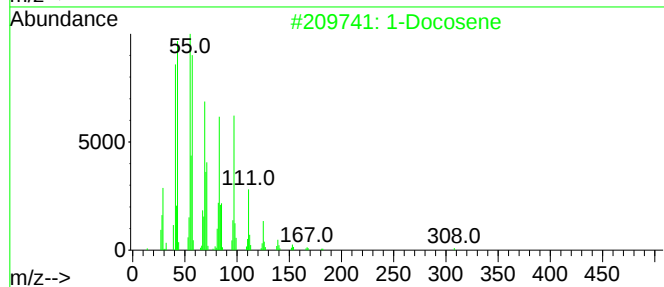
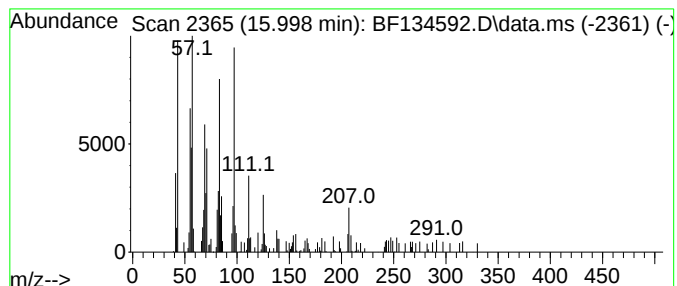
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 1-Docosene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.998	2.48 ng	77383	Perylene-d12	15.421

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Docosene			308	C22H44	001599-67-3	87
2	Triacontan-15-ol			438	C30H62O	031849-26-0	70
3	17-Pentatriacontene			491	C35H70	006971-40-0	62
4	Cyclopentane, 2-isopropyl-1,3-di...			140	C10H20	032281-85-9	53
5	1-Heptacosanol			396	C27H56O	002004-39-9	45



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080223\
Data File : BF134592.D
Acq On : 02 Aug 2023 21:45
Operator : CG\JU
Sample : 03834-02
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
B-P2B

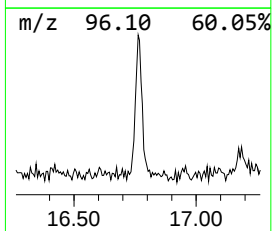
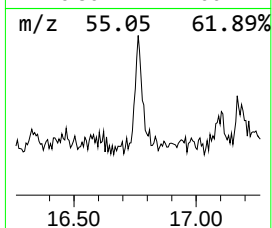
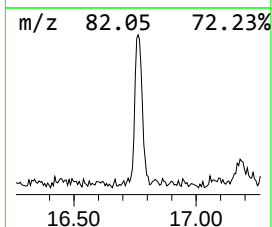
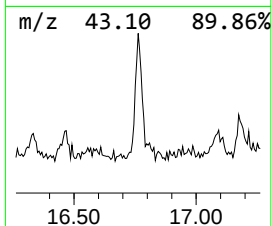
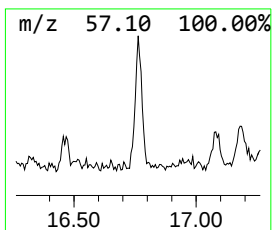
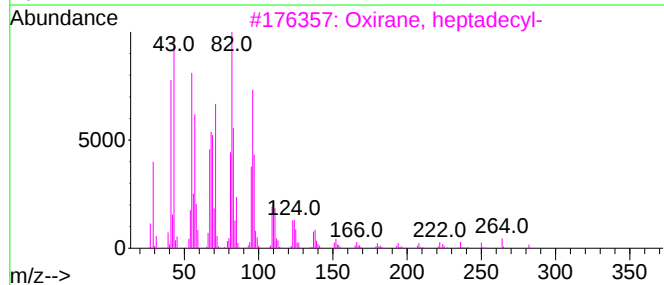
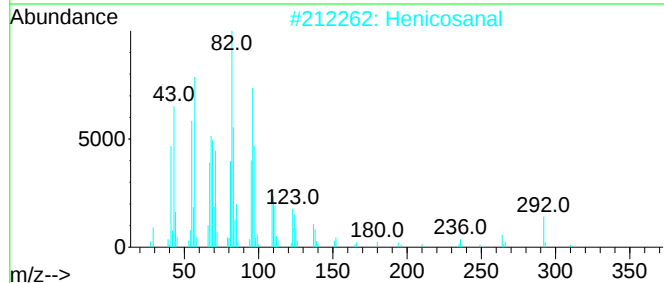
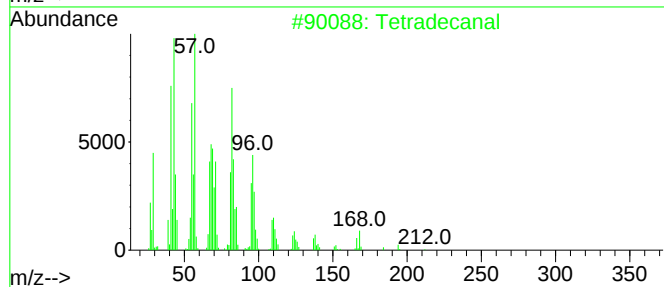
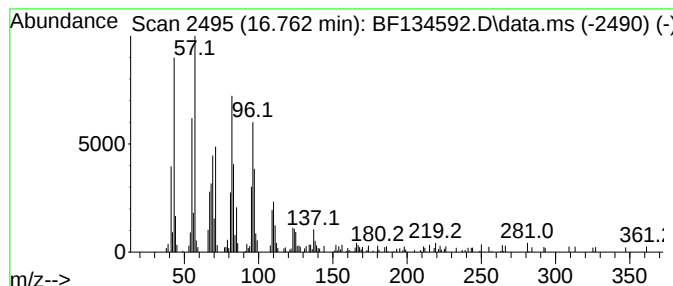
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Tetradecanal Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.762	5.49 ng	171511	Perylene-d12	15.421

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetradecanal	212	C14H28O	000124-25-4	91
2			Henicosanal	310	C21H42O	051227-32-8	87
3			Oxirane, heptadecyl-	282	C19H38O	067860-04-2	87
4			Oxirane, hexadecyl-	268	C18H36O	007390-81-0	81
5			18-Nonadecen-1-ol	282	C19H38O	1000142-89-2	70



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080223\
Data File : BF134592.D
Acq On : 02 Aug 2023 21:45
Operator : CG\JU
Sample : 03834-02
Misc :
ALS Vial : 23 Sample Multiplier: 1

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ClientSampleId :
B-P2B

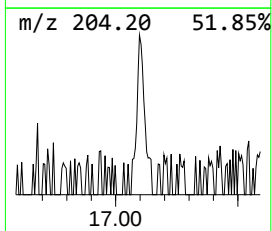
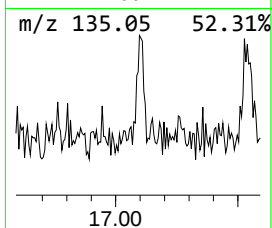
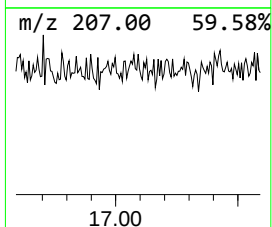
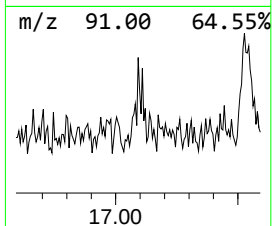
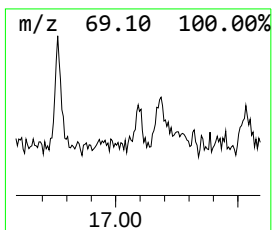
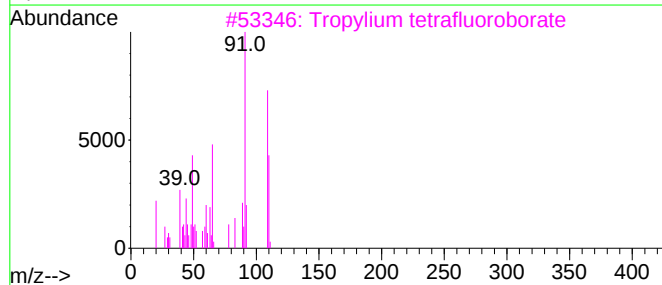
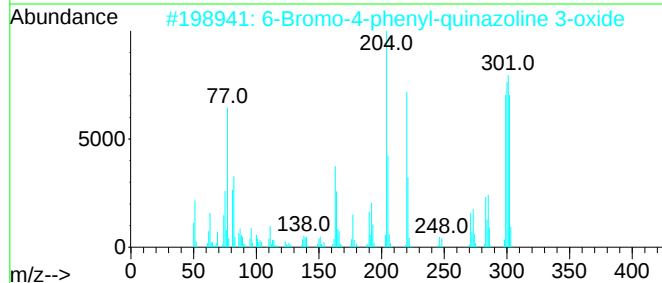
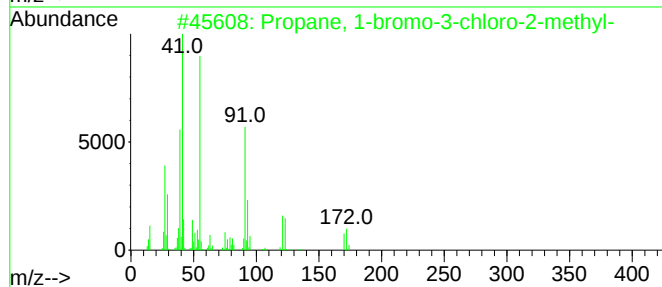
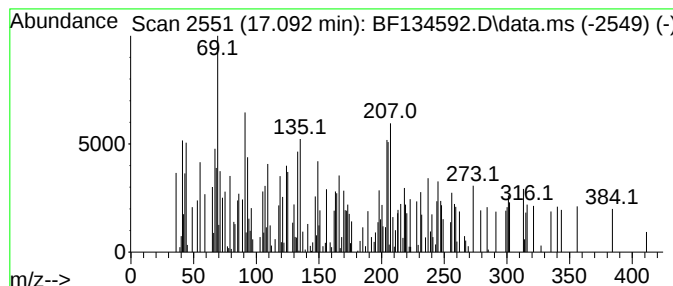
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 unknown17.092 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.092	2.19 ng	68566	Perylene-d12	15.421

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propane, 1-bromo-3-chloro-2-methyl-	170	C4H8BrCl	006974-77-2	14
2			6-Bromo-4-phenyl-quinazoline 3-o...	300	C14H9BrN2O	251639-76-6	11
3			Tropylum tetrafluoroborate	178	C7H7BF4	027081-10-3	10
4			(5-Oxo-2,5-dihydro-1H-pyrrol-3-y...	247	C13H13NO4	1010191-94-5	9
5			3-Aminoxy-4-chlorobutyric acid,...	181	C6H12ClNO3	1000186-78-9	9



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080223\
Data File : BF134592.D
Acq On : 02 Aug 2023 21:45
Operator : CG\JU
Sample : 03834-02
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
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ClientSampleId :
B-P2B

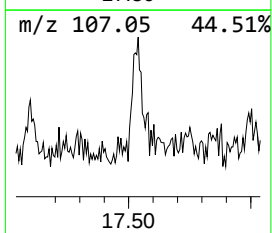
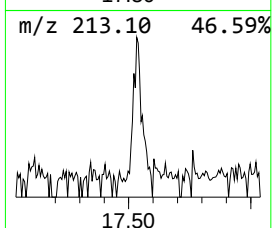
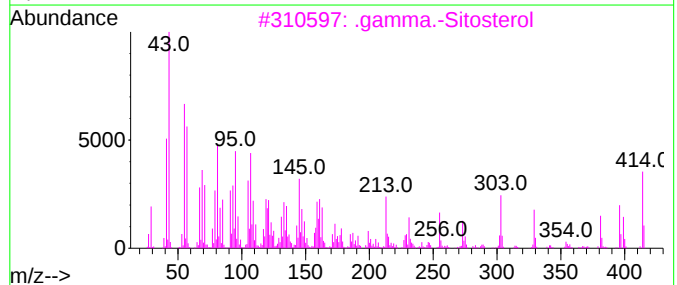
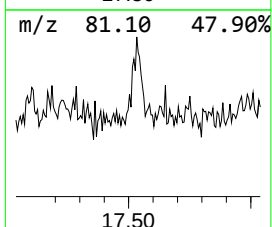
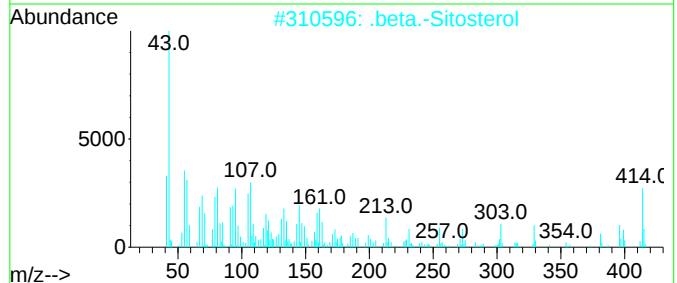
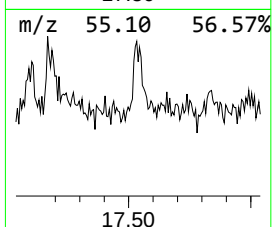
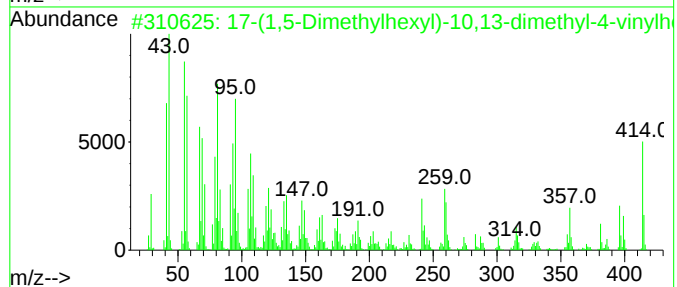
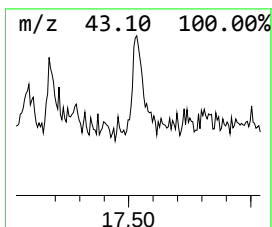
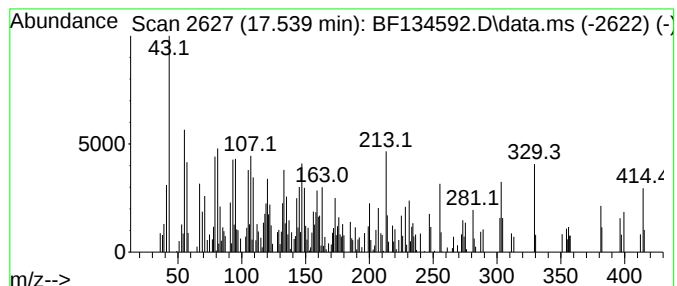
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 17-(1,5-Dimethylhexyl)-10,13-dimethyl-4-vinyl-1,2,3,4,5,6,7,8-octahydro-2H-benzocyclopenta[b]pyridine Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.539	4.82 ng	150711	Perylene-d12	15.421

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	17-(1,5-Dimethylhexyl)-10,13-dimethyl-4-vinyl-1,2,3,4,5,6,7,8-octahydro-2H-benzocyclopenta[b]pyridine	414	C29H50O	1000210-86-9	74		
2	.beta.-Sitosterol	414	C29H50O	000083-46-5	70		
3	.gamma.-Sitosterol	414	C29H50O	000083-47-6	70		
4	.beta.-Sitosterol acetate	456	C31H52O2	000915-05-9	25		
5	Clionasterol acetate	456	C31H52O2	004651-54-1	25		



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080223\
Data File : BF134592.D
Acq On : 02 Aug 2023 21:45
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Sample : 03834-02
Misc :
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Instrument :
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ClientSampleId :
B-P2B

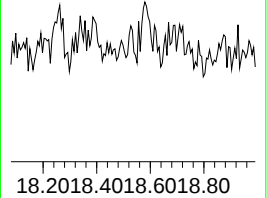
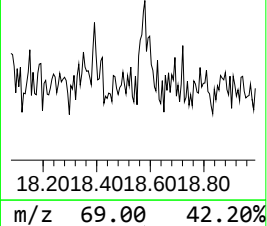
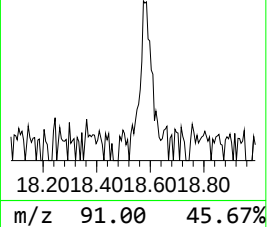
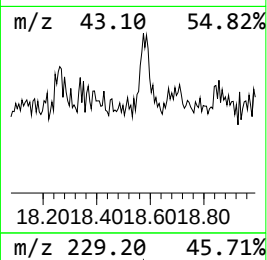
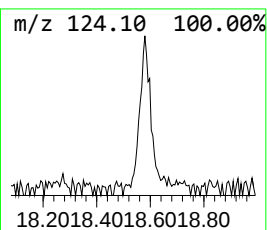
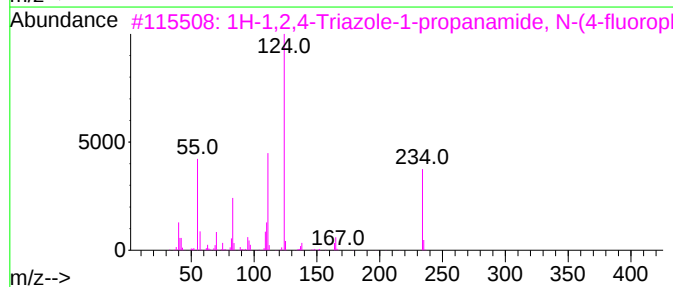
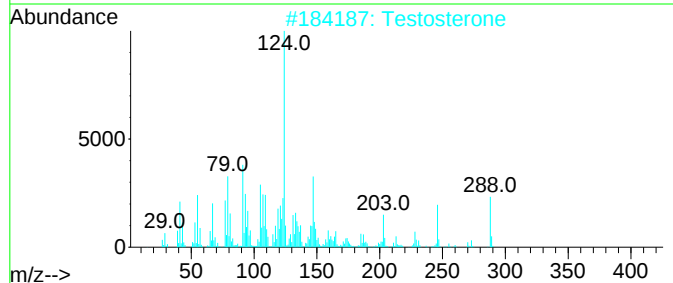
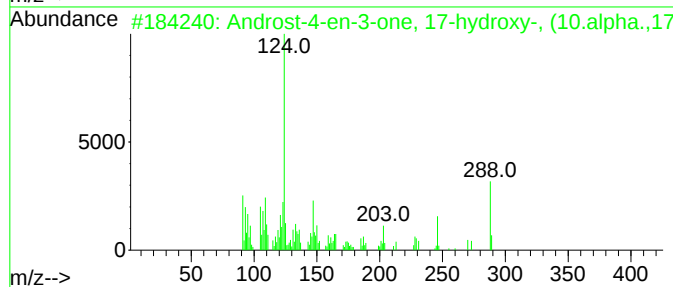
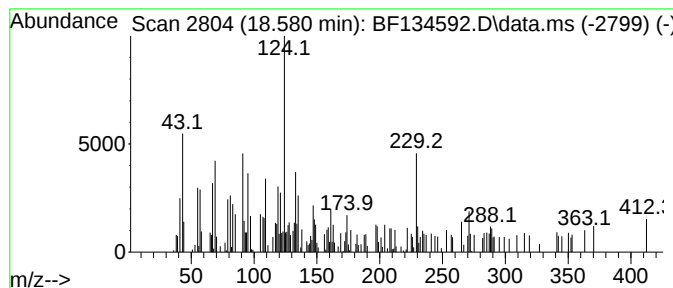
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 unknown18.580 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.580	3.13 ng	97917	Perylene-d12	15.421

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Androst-4-en-3-one, 17-hydroxy-,...	288	C19H28O2	000604-39-7	41
2			Testosterone	288	C19H28O2	000058-22-0	38
3			1H-1,2,4-Triazole-1-propanamide,...	234	C11H11FN4O	1000337-51-7	35
4			3-(3-Fluoroanilino)-1-(3-nitroph...	288	C15H13FN2O3	300726-64-1	35
5			2-Chloro-4-fluorobenzylamide	159	C7H7ClFN	1010343-00-9	30



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080223\
Data File : BF134592.D
Acq On : 02 Aug 2023 21:45
Operator : CG\JU
Sample : 03834-02
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
B-P2B

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

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					#	RT	Resp	Conc
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Supraene	14.833	6.2	ng	192977	6	15.421	624803	20.0
Hexacosane, 1-i...	15.104	2.7	ng	85679	6	15.421	624803	20.0
Oxirane, hexade...	15.698	2.3	ng	72342	6	15.421	624803	20.0
Docosane, 1-iodo-	15.939	2.1	ng	65480	6	15.421	624803	20.0
1-Docosene	15.998	2.5	ng	77383	6	15.421	624803	20.0
Tetradecanal	16.762	5.5	ng	171511	6	15.421	624803	20.0
unknown17.092	17.092	2.2	ng	68566	6	15.421	624803	20.0
17-(1,5-Dimethy...	17.539	4.8	ng	150711	6	15.421	624803	20.0
unknown18.580	18.580	3.1	ng	97917	6	15.421	624803	20.0