LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF070324\
Data File : BF138453.D
Acq On : 03 Jul 2024 18:38
Operator : CG\JU
Sample : P3135-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
OK-628-COMP-01

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-BF062824.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF138453.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	8	14	20	rVB	2090344	2631236	100.00%	13.067%
2	2.275	26	32	41	rVB2	31529	44490	1.69%	0.221%
3	3.393	220	222	234	rBV	45432	98678	3.75%	0.490%
4	5.093	507	511	519	rVB	286862	314753	11.96%	1.563%
5	5.498	576	580	584	rBV	2749040	2527631	96.06%	12.552%
6	6.504	747	751	754	rBV	2478828	2505150	95.21%	12.440%
7	6.698	781	784	789	rVB2	34104	32337	1.23%	0.161%
8	6.869	810	813	817	rBV	897823	715839	27.21%	3.555%
9	7.434	904	909	912	rBV	1859241	1606499	61.05%	7.978%
10	8.151	1027	1031	1034	rVB	1136194	848881	32.26%	4.215%
11	8.463	1081	1084	1087	rBV	52040	46197	1.76%	0.229%
12	9.228	1209	1214	1217	rBV	2947166	2354109	89.47%	11.690%
13	9.904	1325	1329	1332	rBV	932305	720189	27.37%	3.576%
14	9.998	1341	1345	1351	rVB2	35350	50738	1.93%	0.252%
15	10.692	1459	1463	1466	rBV	1233194	999611	37.99%	4.964%
16	10.804	1479	1482	1487	rBV2	32431	42381	1.61%	0.210%
17	11.122	1532	1536	1539	rVB	36095	38065	1.45%	0.189%
18	11.392	1578	1582	1584	rBV	657747	600130	22.81%	2.980%
19	11.916	1668	1671	1676	rBV	246200	235622	8.95%	1.170%
20	12.474	1763	1766	1772	rVB2	28702	36109	1.37%	0.179%
21	12.598	1785	1787	1793	rBV	39710	41854	1.59%	0.208%
22	12.698	1801	1804	1810	rBV	109695	126543	4.81%	0.628%
23	12.827	1824	1826	1832	rVB2	46016	63916	2.43%	0.317%
24	12.974	1847	1851	1854	rBV	2237954	1926288	73.21%	9.566%
25	13.204	1887	1890	1895	rVB	31470	30626	1.16%	0.152%
26	13.545	1945	1948	1951	rBV	37902	32782	1.25%	0.163%
27	13.874	2000	2004	2013	rVB	162480	222694	8.46%	1.106%
28	14.027	2026	2030	2033	rBV	623760	545037	20.71%	2.707%
29	14.186	2055	2057	2065	rVB	51184	51721	1.97%	0.257%
30	14.492	2107	2109	2112	rBV	57222	40781	1.55%	0.203%
31	14.786	2156	2159	2160	rBV	44660	48837	1.86%	0.243%
32	15.492	2275	2279	2289	rVB2	281864	392489	14.92%	1.949%
33	16.204	2397	2400	2410	rVB6	54878	102197	3.88%	0.508%
34	16.633	2471	2473	2482	rVB3	39452	62834	2.39%	0.312%

Sum of corrected areas: 20137244

Instrument :
BNA_F
ClientSampleId :
OK-628-COMP-01

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF070324\
Data File : BF138453.D
Acq On : 03 Jul 2024 18:38
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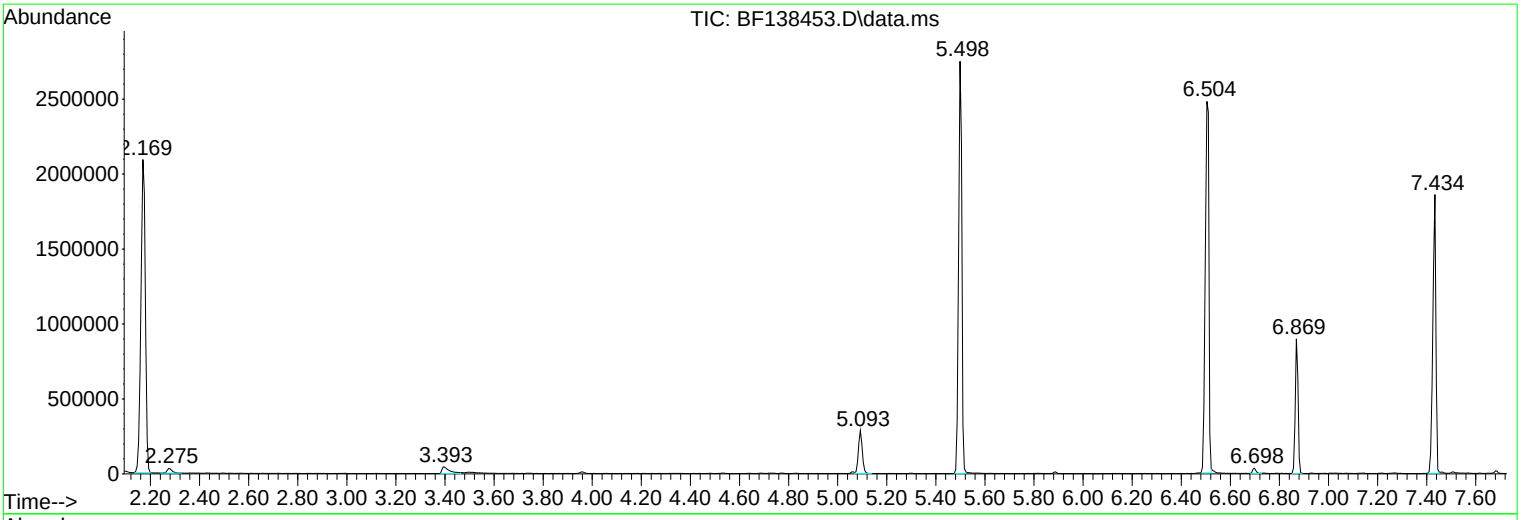
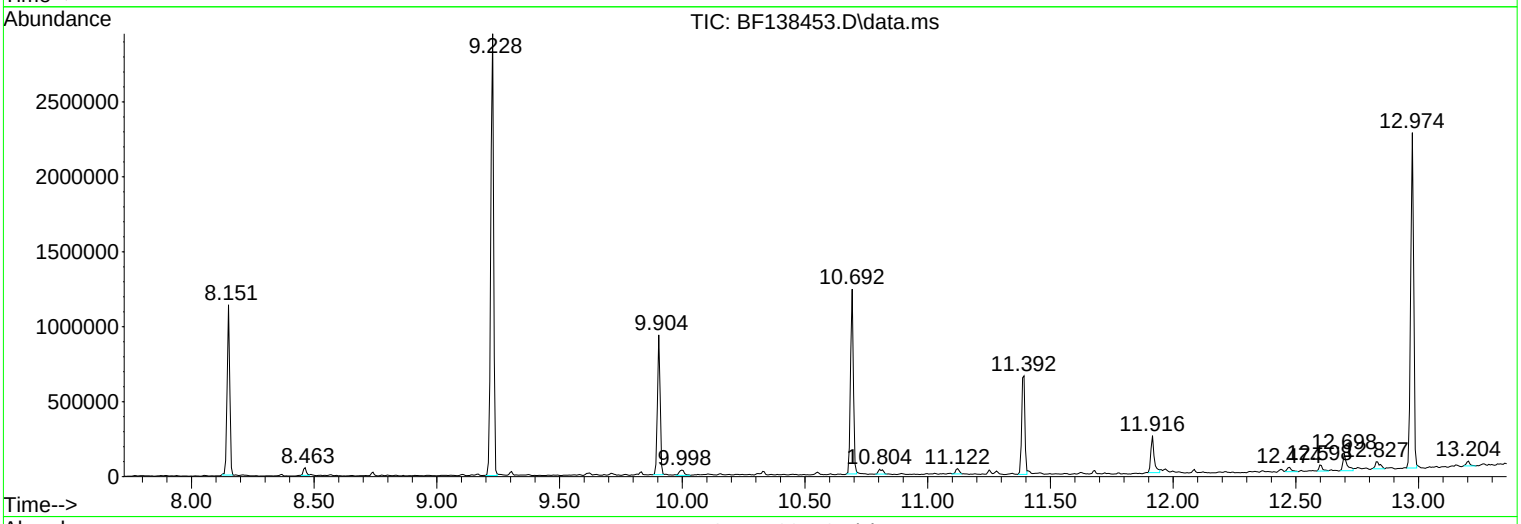
Sample : P3135-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

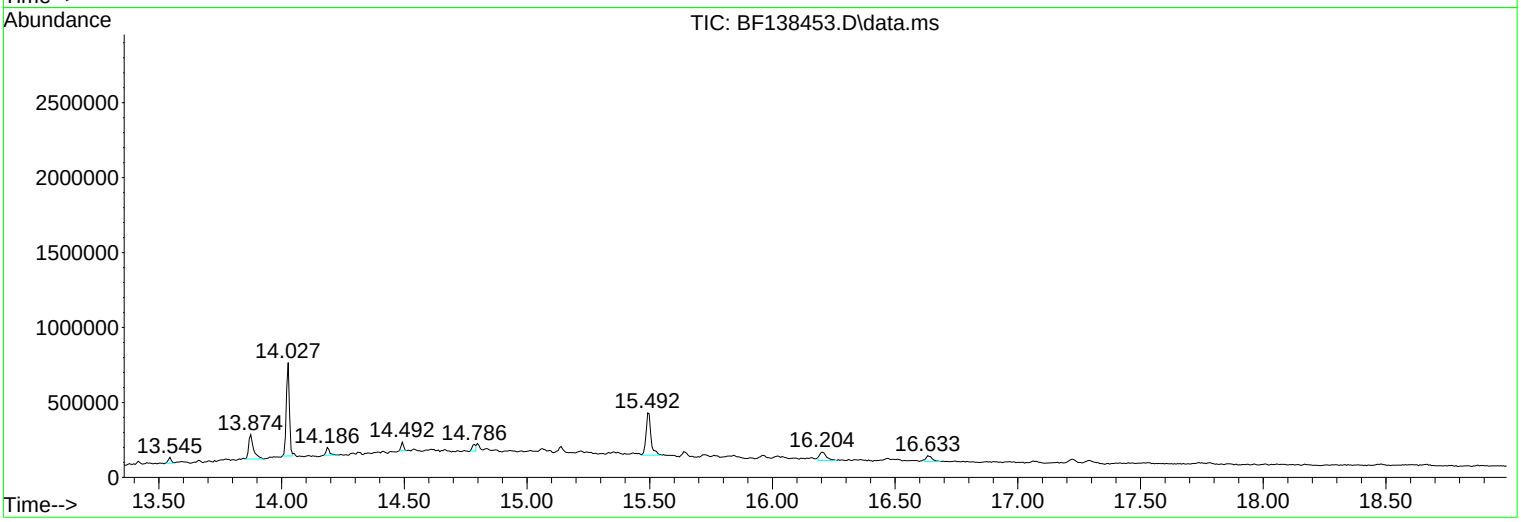
Instrument :
BNA_F
ClientSampleId :
OK-628-COMP-01

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062824.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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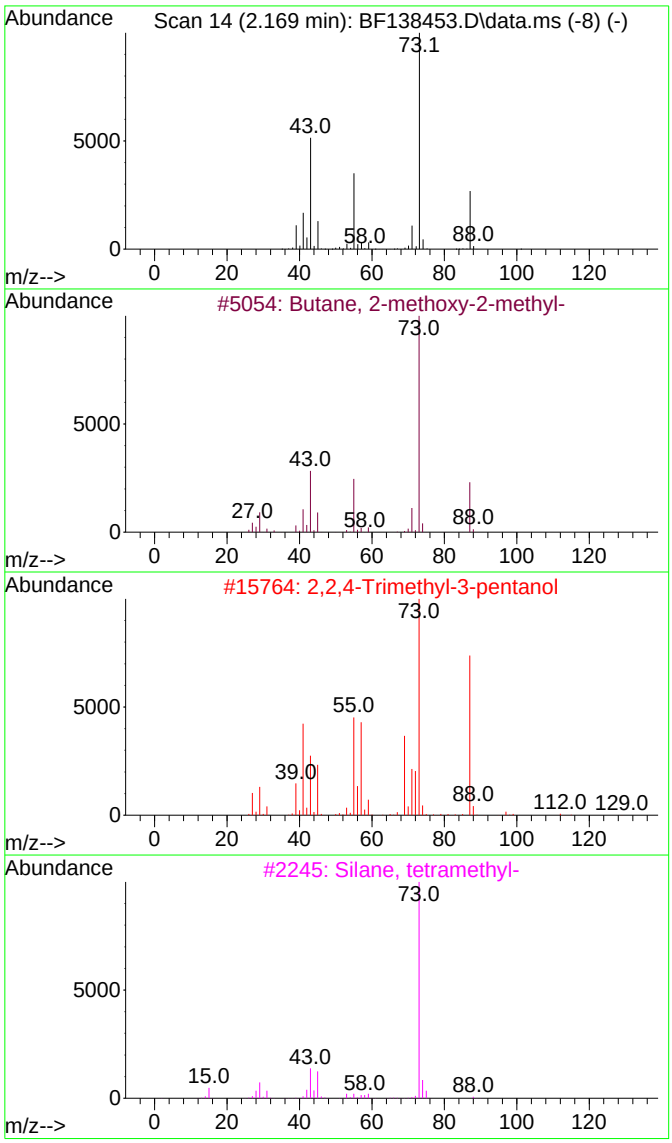
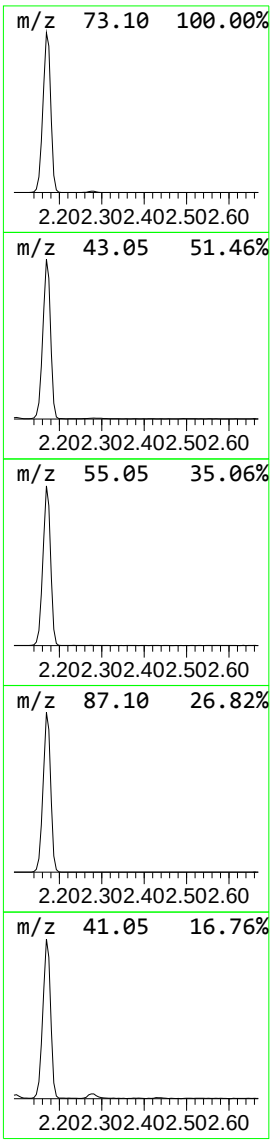
****
Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.169	73.51 ng	2631240	1,4-Dichlorobenzene-d4	6.869

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3	Silane, tetramethyl-	88	C4H12Si	000075-76-3	38
4	3-Pentanol, 3-methyl-	102	C6H14O	000077-74-7	23
5	Borane, dimethoxy-	74	C2H7BO2	004542-61-4	9





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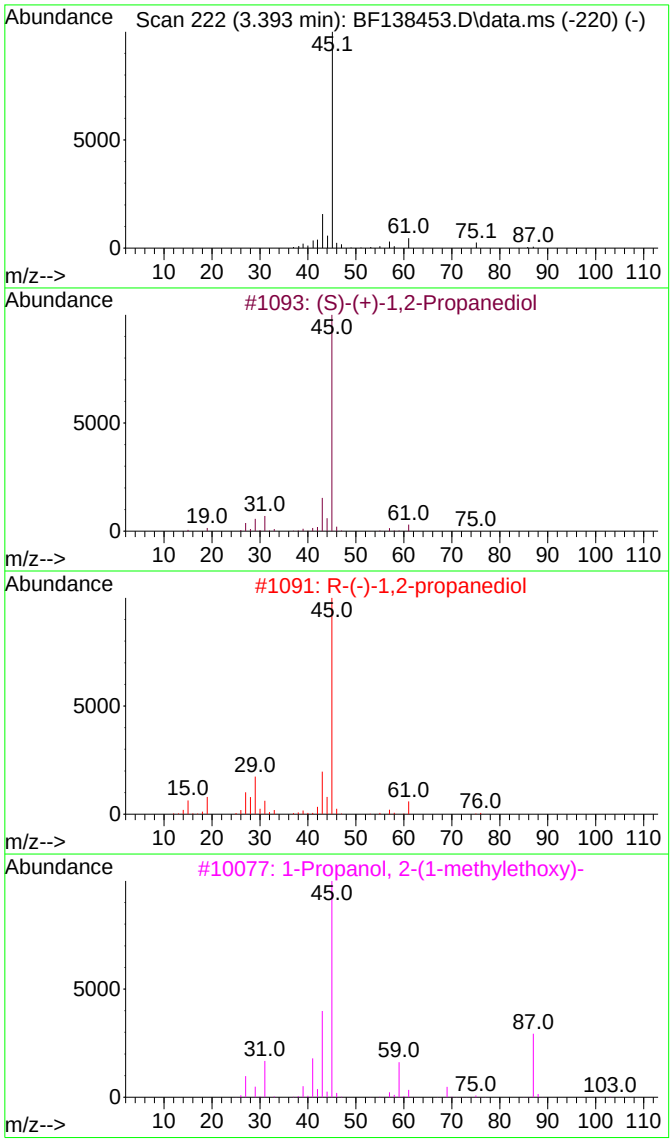
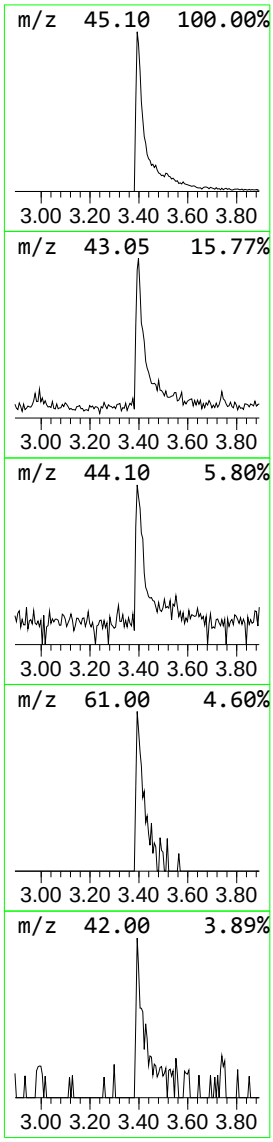
****

Peak Number 2 unknown3.393 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.393	2.76 ng	98678	1,4-Dichlorobenzene-d4	6.869

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	40
2	R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	40
3	1-Propanol, 2-(1-methylethoxy)-	118	C6H14O2	003944-37-4	9
4	2,3-Butanediol	90	C4H10O2	000513-85-9	9
5	Propylene Glycol	76	C3H8O2	000057-55-6	9





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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062824.M
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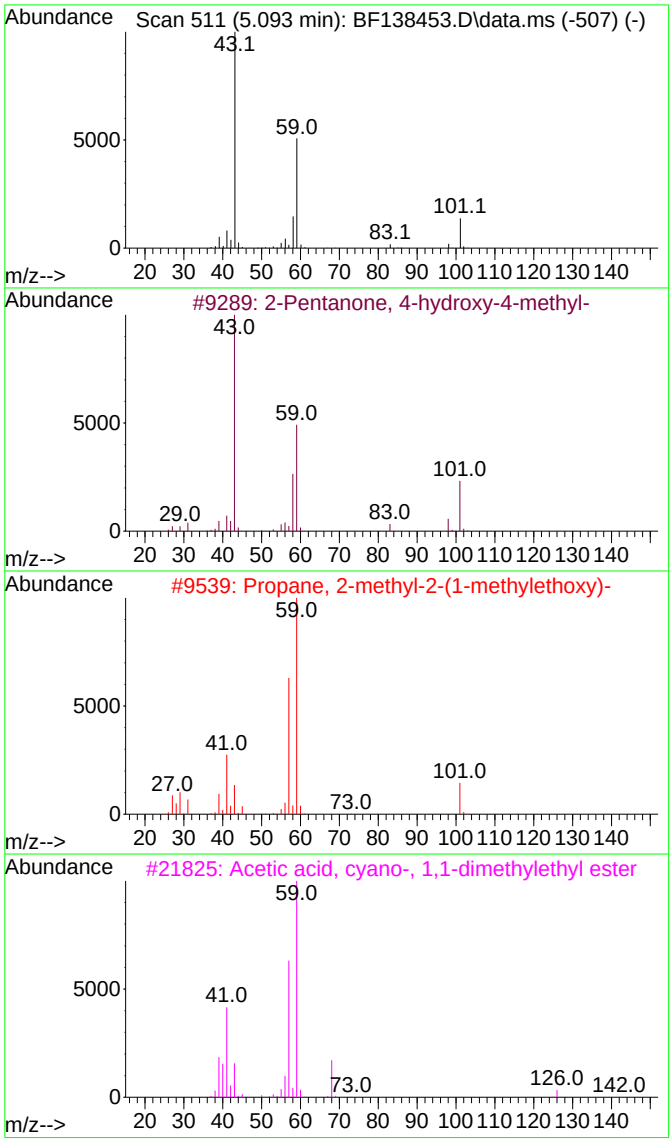
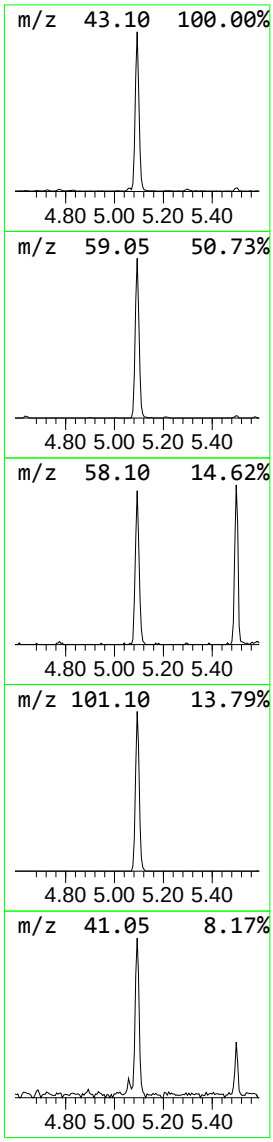
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.093	8.79 ng	314753	1,4-Dichlorobenzene-d4	6.869

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16
5	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	9





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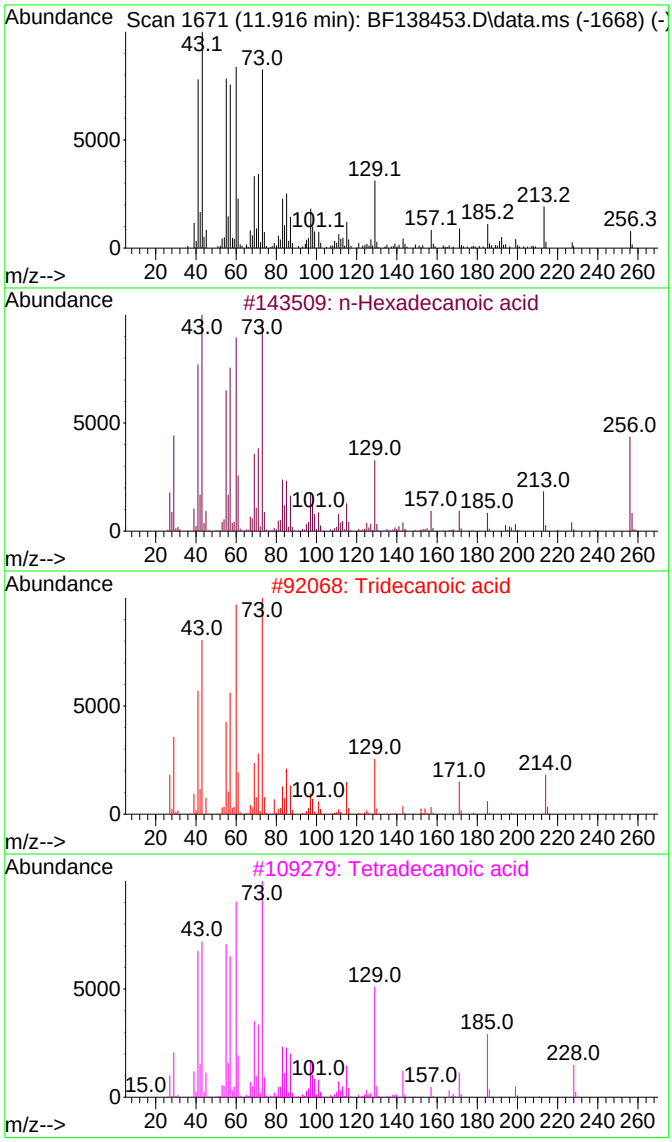
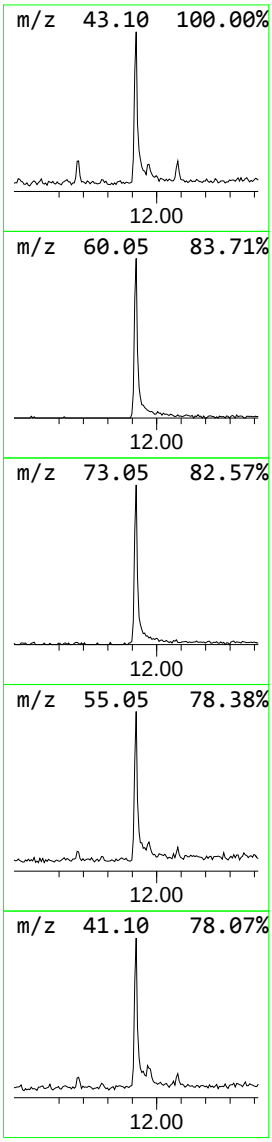
****

Peak Number 4 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.916	7.85 ng	235622	Phenanthrene-d10	11.392

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	96
2	Tridecanoic acid	214	C13H26O2	000638-53-9	81
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	72
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	68
5	Undecanoic acid	186	C11H22O2	000112-37-8	64





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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062824.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

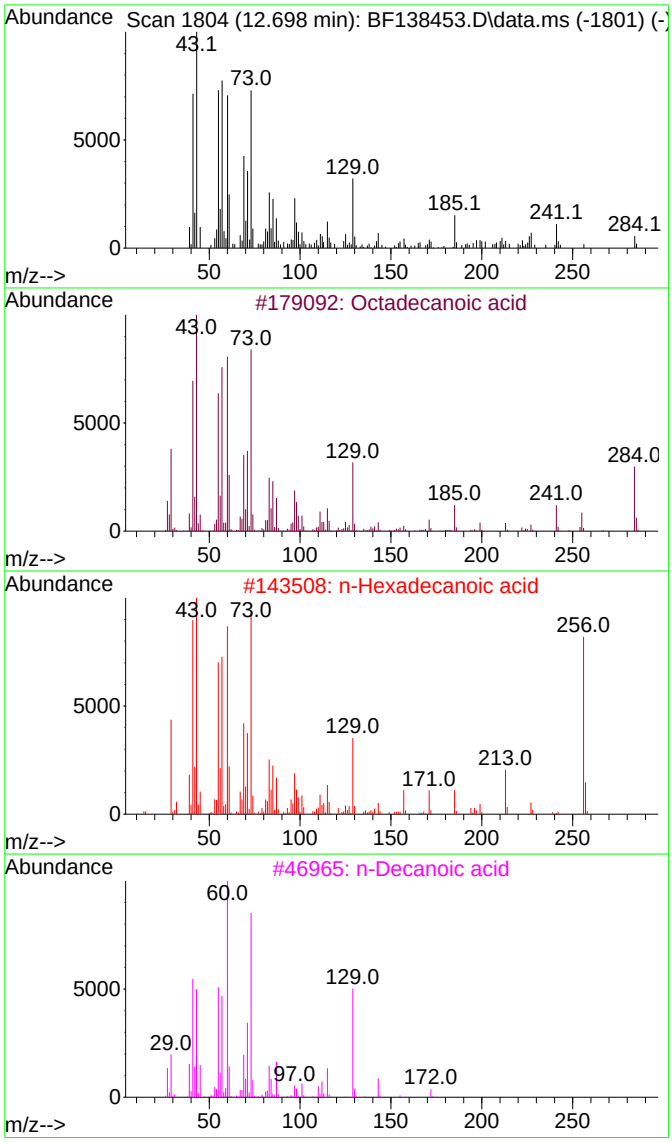
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

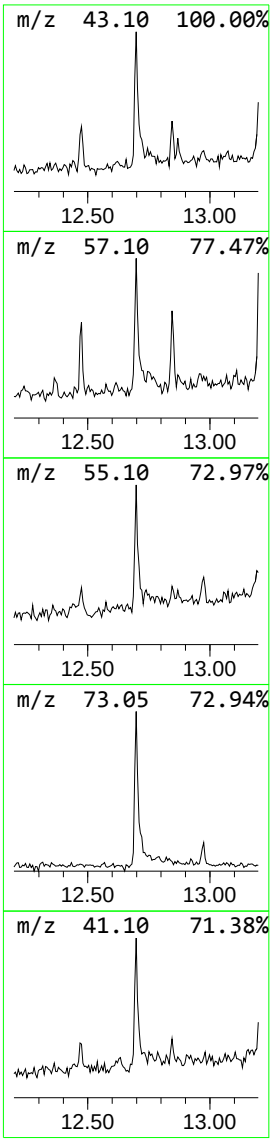
****

Peak Number 5 Octadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.698	4.22 ng	126543	Phenanthrene-d10	11.392

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	95
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	86
3	n-Decanoic acid	172	C10H20O2	000334-48-5	60
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	58
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	52





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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062824.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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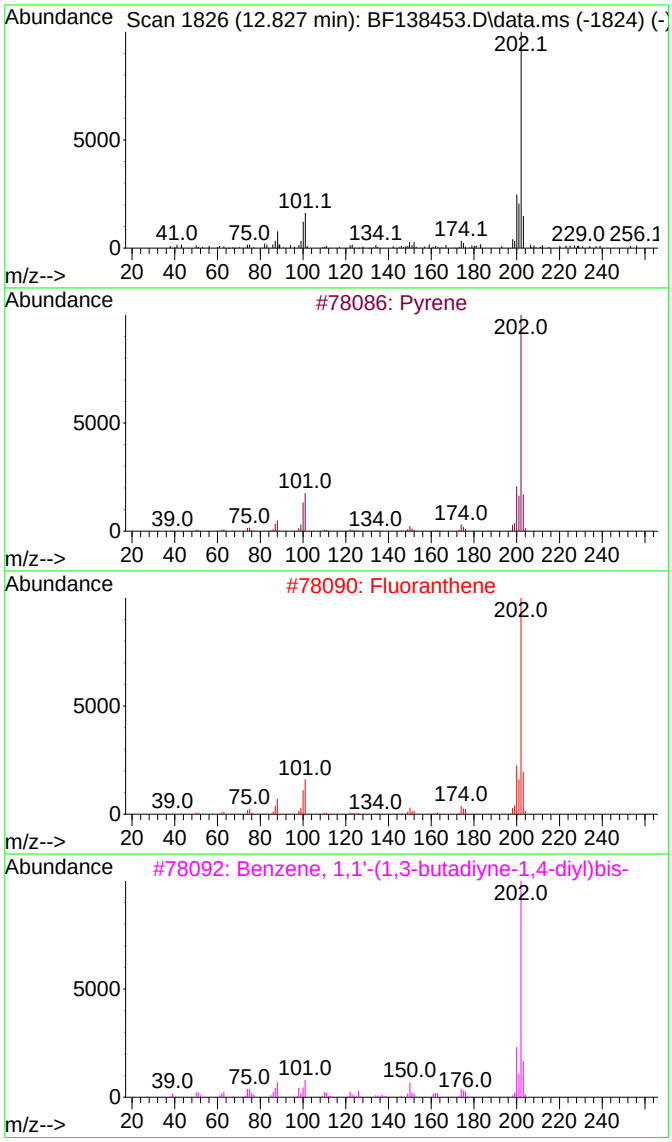
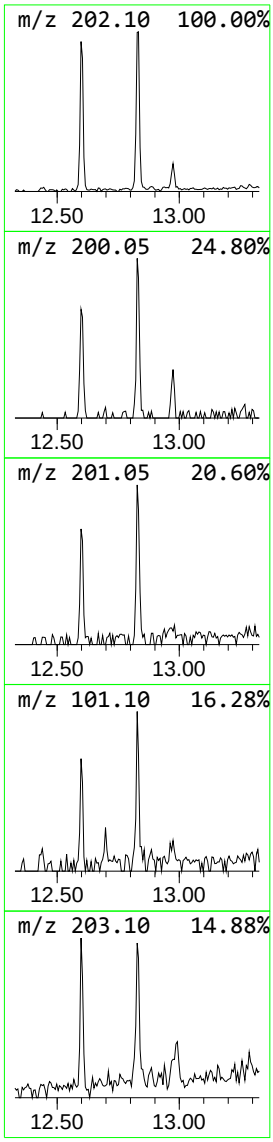
****
Peak Number 6 Benzene, 1,1'-(1,3-butadiyn... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.827	2.35 ng	63916	Chrysene-d12	14.027

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pyrene	202	C16H10	000129-00-0	96
2	Fluoranthene	202	C16H10	000206-44-0	94
3	Benzene, 1,1'-(1,3-butadiyne-1,4...	202	C16H10	000886-66-8	52
4	1-Methyl-7,11-dithiaspiro[5,5] u...	202	C10H18S2	107678-22-8	38
5	4-Methoxy-naphthalene-1-carboxyl...	202	C12H10O3	1000317-85-4	37





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TIC Library : C:\Database\NIST20.L
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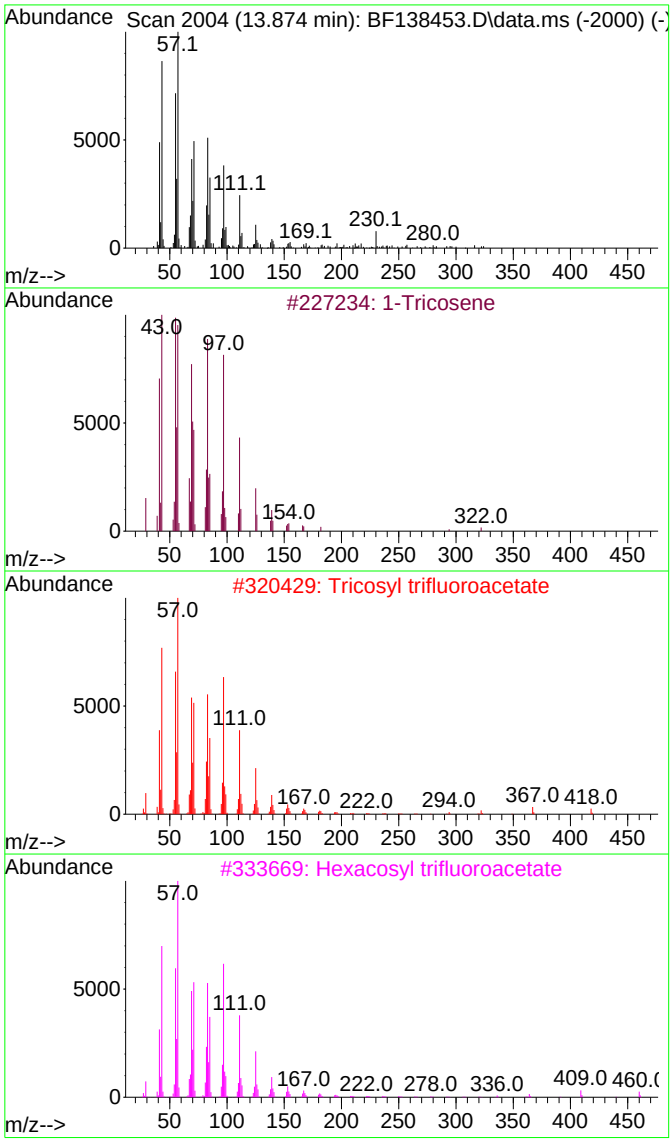
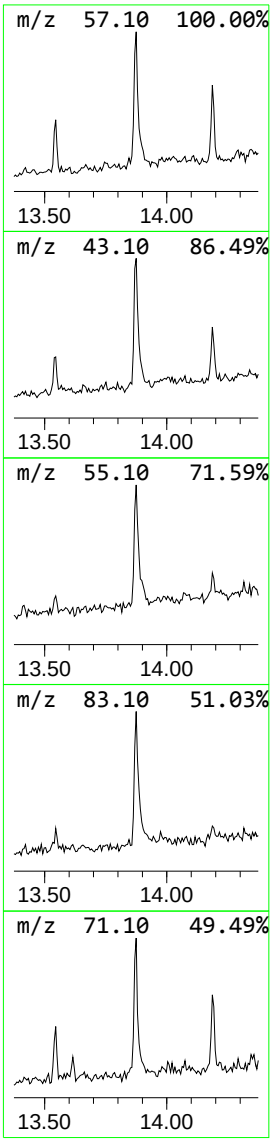
Peak Number 7 1-Tricosene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.874	8.17 ng	222694	Chrysene-d12	14.027

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Tricosene	322	C23H46	018835-32-0	95
2	Tricosyl trifluoroacetate	436	C25H47F3O2	1000351-75-1	91
3	Hexacosyl trifluoroacetate	478	C28H53F3O2	1000351-75-0	91
4	Tricosyl heptafluorobutyrate	536	C27H47F7O2	1000351-83-4	91
5	Hexacosyl heptafluorobutyrate	578	C30H53F7O2	1000351-83-3	91





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TIC Library : C:\Database\NIST20.L
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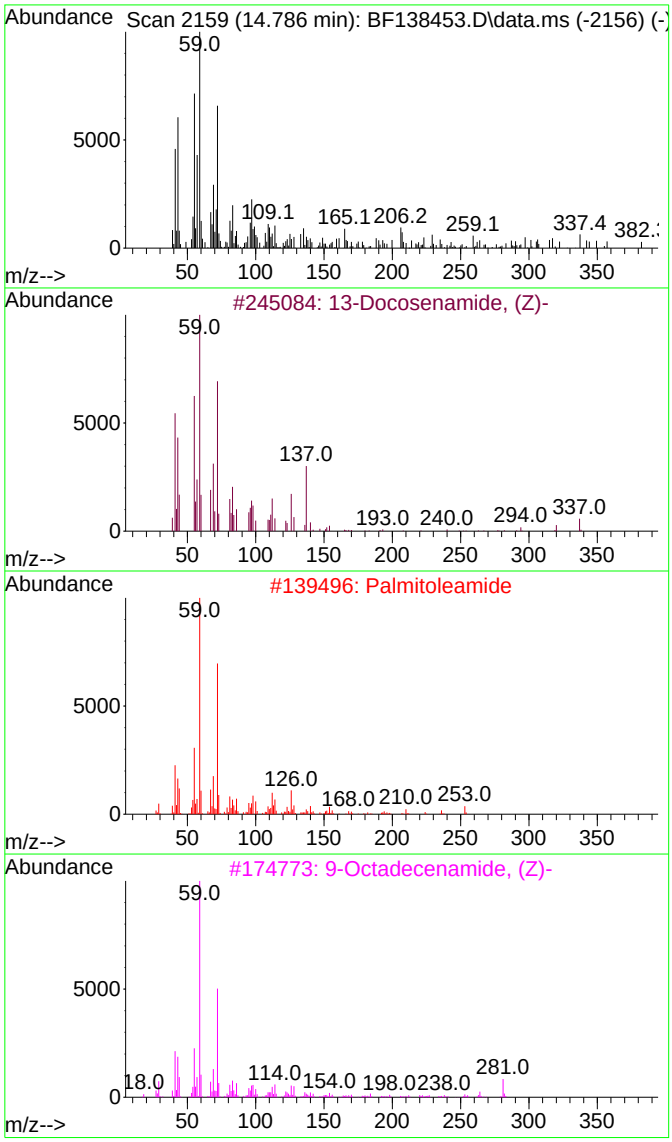
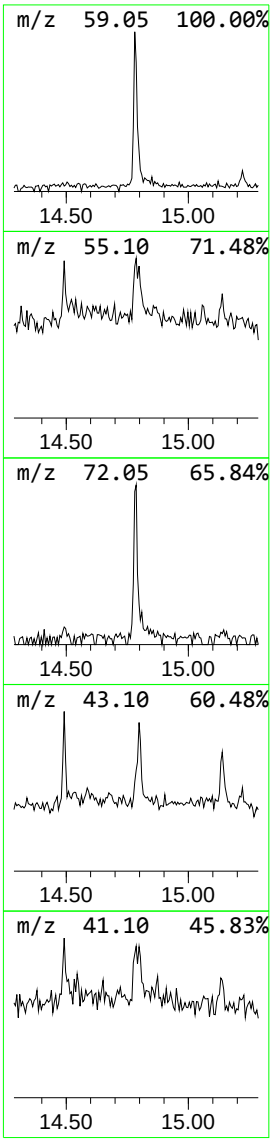
Peak Number 8 13-Docosenamide, (Z)- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.786	2.49 ng	48837	Perylene-d12	15.498

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	13-Docosenamide, (Z)-	337	C22H43NO	000112-84-5	93
2	Palmitoleamide	253	C16H31NO	106010-22-4	53
3	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	53
4	Octadecanamide	283	C18H37NO	000124-26-5	46
5	Cyclohexanecarboxamide	127	C7H13NO	001122-56-1	27





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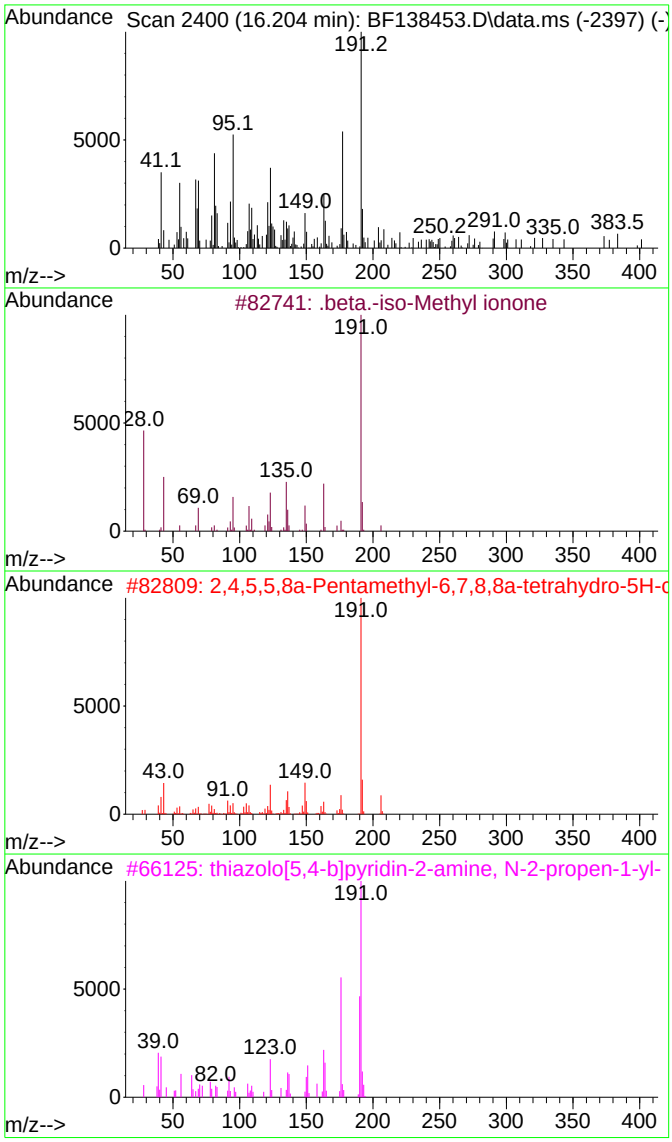
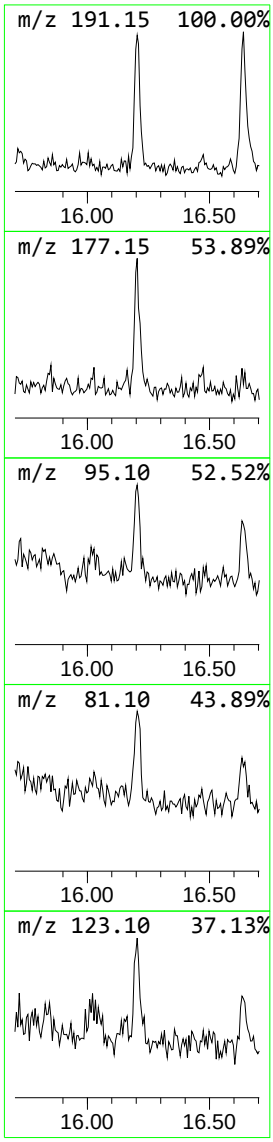
****

Peak Number 9 .beta.-iso-Methyl ionone Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.204	5.21 ng	102197	Perylene-d12	15.498

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	.beta.-iso-Methyl ionone	206	C14H22O	1000285-40-2	70
2	2,4,5,5,8a-Pentamethyl-6,7,8,8a-...	206	C14H22O	1000195-40-9	52
3	thiazolo[5,4-b]pyridin-2-amine, ...	191	C9H9N3S	1000400-23-3	50
4	1-Penten-3-one, 1-(2,6,6-trimeth...	206	C14H22O	000127-43-5	45
5	Spiro[4-oxatricyclo[5.3.0.0(2,6)...	276	C18H28O2	1000156-82-9	43





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF070324\
Data File : BF138453.D
Acq On : 03 Jul 2024 18:38
Operator : CG\JU
Sample : P3135-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
OK-628-COMP-01

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062824.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

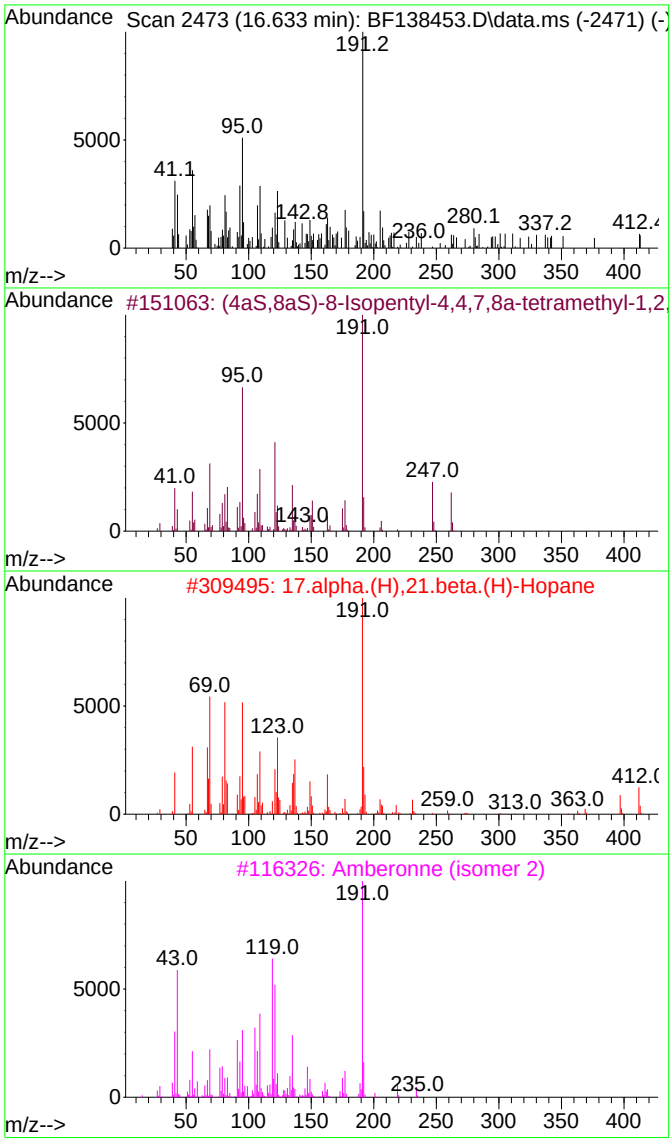
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

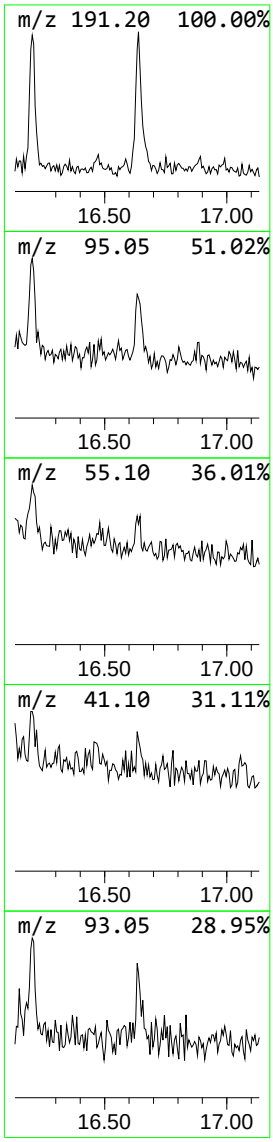
****

Peak Number 10 (4aS,8aS)-8-Isopentyl-4,4,7... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.633	3.20 ng	62834	Perylene-d12	15.498

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(4aS,8aS)-8-Isopentyl-4,4,7,8a-t...	262	C19H34	220766-79-0	81
2	17.alpha.(H),21.beta.(H)-Hopane	412	C30H52	013849-96-2	59
3	Amberonne (isomer 2)	234	C16H26O	1010470-69-8	58
4	1-Cyclohexene, 1,3,3-trimethyl-2...	206	C14H22O	1000197-08-4	53
5	2-Furoic acid, 2-methyloct-5-yn-...	234	C14H18O3	1000299-23-7	47





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF070324\
Data File : BF138453.D
Acq On : 03 Jul 2024 18:38
Operator : CG\JU
Sample : P3135-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
OK-628-COMP-01

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062824.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Butane, 2-metho...	2.169	73.5	ng	2631240	1	6.869	715839	20.0
unknown3.393	3.393	2.8	ng	98678	1	6.869	715839	20.0
2-Pentanone, 4-...	5.093	8.8	ng	314753	1	6.869	715839	20.0
n-Hexadecanoic ...	11.916	7.8	ng	235622	4	11.392	600130	20.0
Octadecanoic acid	12.698	4.2	ng	126543	4	11.392	600130	20.0
Benzene, 1,1'-(...	12.827	2.4	ng	63916	5	14.027	545037	20.0
1-Tricosene	13.874	8.2	ng	222694	5	14.027	545037	20.0
13-Docosenamide...	14.786	2.5	ng	48837	6	15.498	392489	20.0
.beta.-iso-Meth...	16.204	5.2	ng	102197	6	15.498	392489	20.0
(4aS,8aS)-8-Iso...	16.633	3.2	ng	62834	6	15.498	392489	20.0