LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF042624\
Data File : BF137735.D
Acq On : 26 Apr 2024 15:16
Operator : CG\JU
Sample : P2218-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
B-131-GW-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-BF042324.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF137735.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.222	16	23	28	rVB3	127400	240626	3.44%	0.503%
2	2.434	53	59	66	rVB	1126268	1443852	20.62%	3.018%
3	5.299	538	546	550	rBV	68480	72362	1.03%	0.151%
4	5.675	606	610	614	rBV	2885848	2699200	38.55%	5.641%
5	6.346	721	724	728	rVB	222322	181631	2.59%	0.380%
6	6.610	761	769	773	rBV	63502	96766	1.38%	0.202%
7	6.663	773	778	781	rBV	2015732	1783288	25.47%	3.727%
8	7.057	842	845	849	rBV	1787908	1562668	22.32%	3.266%
9	7.587	930	935	937	rBV	134549	147376	2.10%	0.308%
10	7.622	937	941	944	rVB	3961411	3642564	52.03%	7.613%
11	7.822	972	975	977	rVV	138361	96499	1.38%	0.202%
12	7.851	977	980	987	rVB2	226858	246308	3.52%	0.515%
13	8.075	1015	1018	1021	rBV	205457	162063	2.31%	0.339%
14	8.234	1042	1045	1050	rBV	110608	118243	1.69%	0.247%
15	8.345	1058	1064	1070	rBV	2449461	2353196	33.61%	4.918%
16	8.645	1113	1115	1122	rVB	66038	81247	1.16%	0.170%
17	8.928	1160	1163	1166	rBV	116477	90481	1.29%	0.189%
18	9.057	1179	1185	1188	rBV	215017	192985	2.76%	0.403%
19	9.157	1197	1202	1205	rVB	374368	319354	4.56%	0.667%
20	9.416	1241	1246	1250	rBV	7254010	7001287	100.00%	14.632%
21	9.681	1285	1291	1295	rBV2	202603	285708	4.08%	0.597%
22	9.757	1300	1304	1306	rBV	390324	358978	5.13%	0.750%
23	9.781	1306	1308	1311	rVB	178782	153982	2.20%	0.322%
24	9.875	1321	1324	1329	rBV	157935	176576	2.52%	0.369%
25	10.104	1359	1363	1366	rBV	3031161	2383905	34.05%	4.982%
26	10.134	1366	1368	1372	rVB	1035786	909170	12.99%	1.900%
27	10.263	1384	1390	1392	rBV2	57684	74195	1.06%	0.155%
28	10.310	1394	1398	1401	rVB	500954	468781	6.70%	0.980%
29	10.510	1427	1432	1438	rVB3	64641	101134	1.44%	0.211%
30	10.651	1452	1456	1460	rVB	723622	602425	8.60%	1.259%
31	10.810	1481	1483	1487	rVB	111723	90335	1.29%	0.189%
32	10.892	1493	1497	1501	rBV	4115793	4009161	57.26%	8.379%
33	11.022	1516	1519	1524	rVB2	170276	168356	2.40%	0.352%
34	11.198	1543	1549	1552	rBV3	47505	71557	1.02%	0.150%
35	11.598	1613	1617	1620	rBV	2753285	2456115	35.08%	5.133%
36	11.622	1620	1621	1624	rVB	506565	288720	4.12%	0.603%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF042624\
Data File : BF137735.D
Acq On : 26 Apr 2024 15:16
Operator : CG\JU
Sample : P2218-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
B-131-GW-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-BF042324.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	11.692	1632	1633	1639	rVB2	94240	98261	1.40%	0.205%
38	11.822	1652	1655	1662	rBV	90469	106721	1.52%	0.223%
39	12.104	1697	1703	1709	rBV	926099	1012555	14.46%	2.116%
40	12.216	1718	1722	1724	rBV2	81426	85810	1.23%	0.179%
41	12.816	1819	1824	1829	rBV	123468	128162	1.83%	0.268%
42	12.892	1833	1837	1849	rVV	470134	453353	6.48%	0.947%
43	12.986	1849	1853	1858	rBV	924292	844002	12.05%	1.764%
44	13.186	1883	1887	1891	rBV	7302137	6747365	96.37%	14.102%
45	14.080	2035	2039	2050	rBV	288686	445540	6.36%	0.931%
46	14.245	2064	2067	2071	rBV	1514283	1363946	19.48%	2.851%
47	15.122	2213	2216	2220	rBV	77665	80819	1.15%	0.169%
48	15.821	2329	2335	2348	rBV	1046461	1350273	19.29%	2.822%

Sum of corrected areas: 47847901

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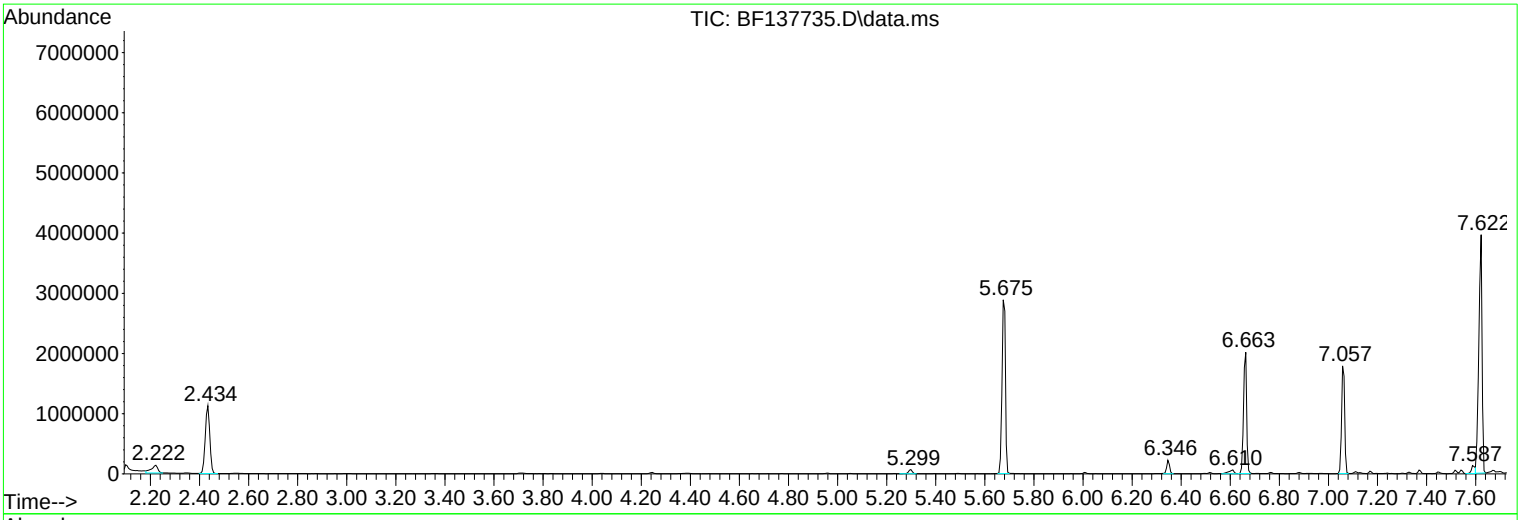
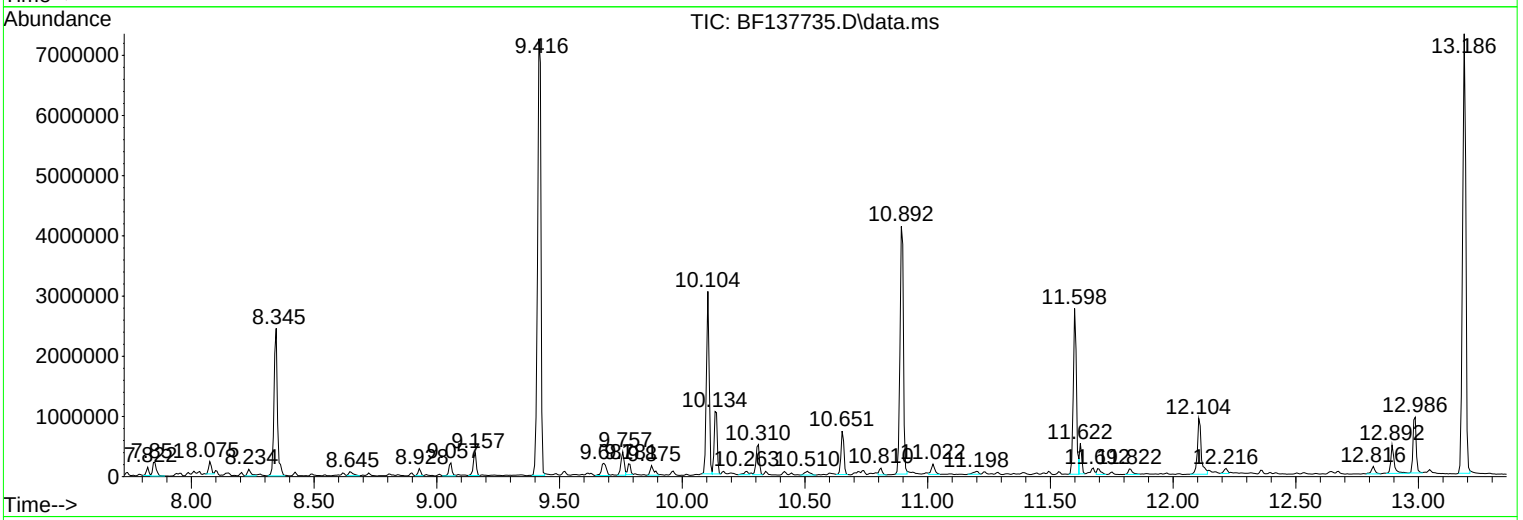
Data File : BF137735.D
Acq On : 26 Apr 2024 15:16
Operator : CG\JU
Sample : P2218-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

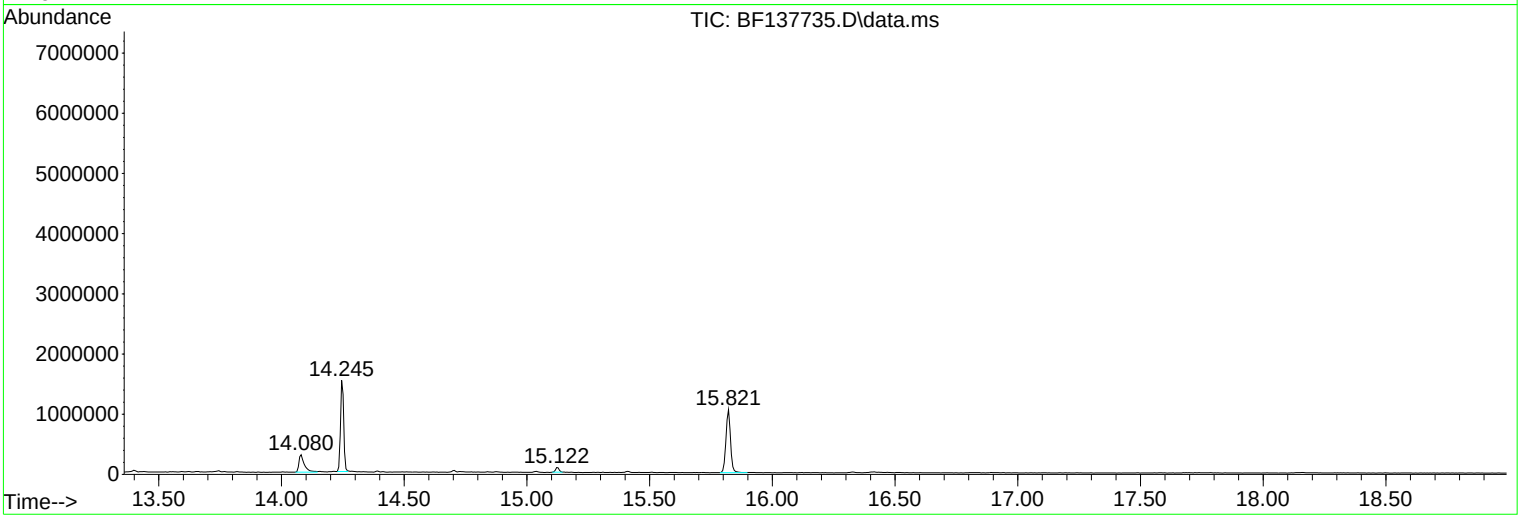
Instrument :
BNA_F
ClientSampleId :
B-131-GW-01

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042324.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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







Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF042624\
Data File : BF137735.D
Acq On : 26 Apr 2024 15:16
Operator : CG\JU
Sample : P2218-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
B-131-GW-01

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042324.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

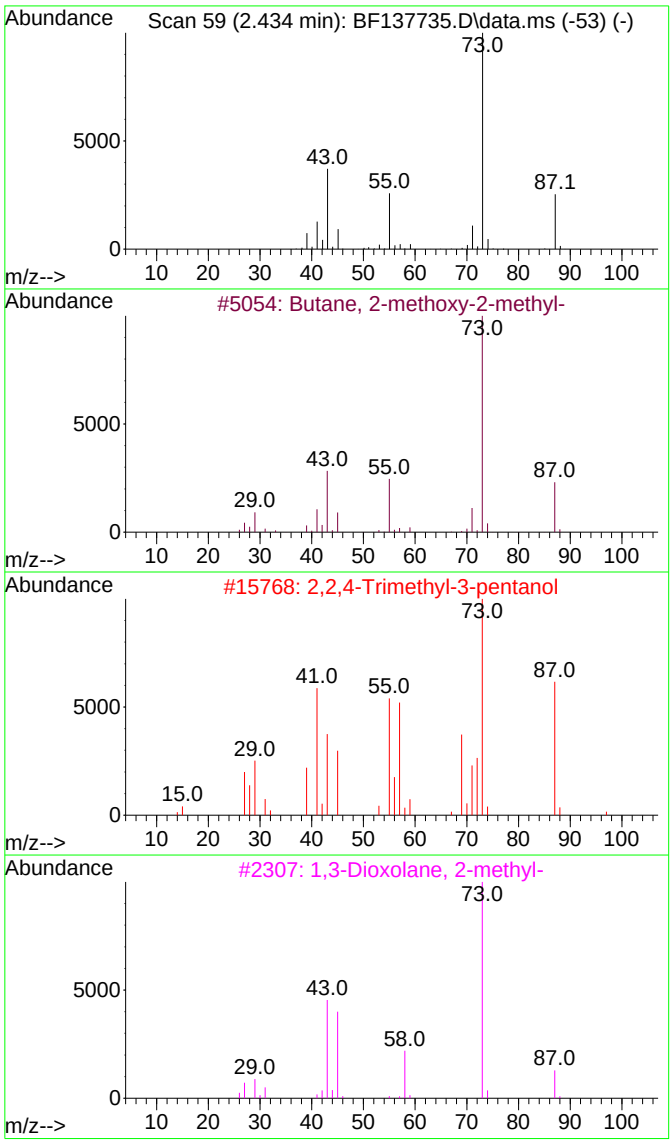
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

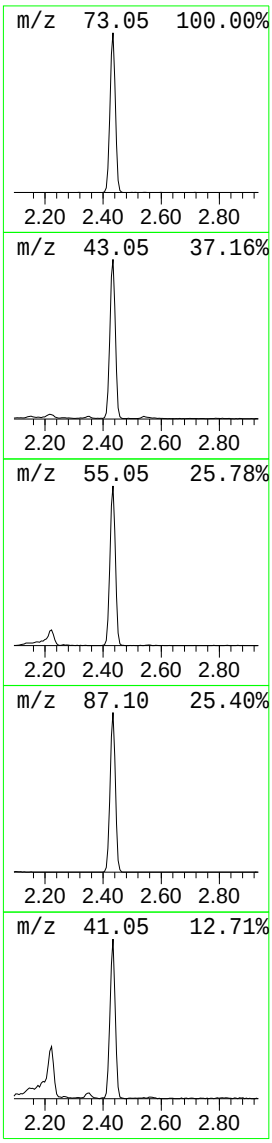
****

Peak Number 2 Butane, 2-methoxy-2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.434	18.48 ng	1443850	1,4-Dichlorobenzene-d4	7.057

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	40
3	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	37
4	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17
5	Silane, tetramethyl-	88	C4H12Si	000075-76-3	12





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF042624\
Data File : BF137735.D
Acq On : 26 Apr 2024 15:16
Operator : CG\JU
Sample : P2218-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
B-131-GW-01

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042324.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

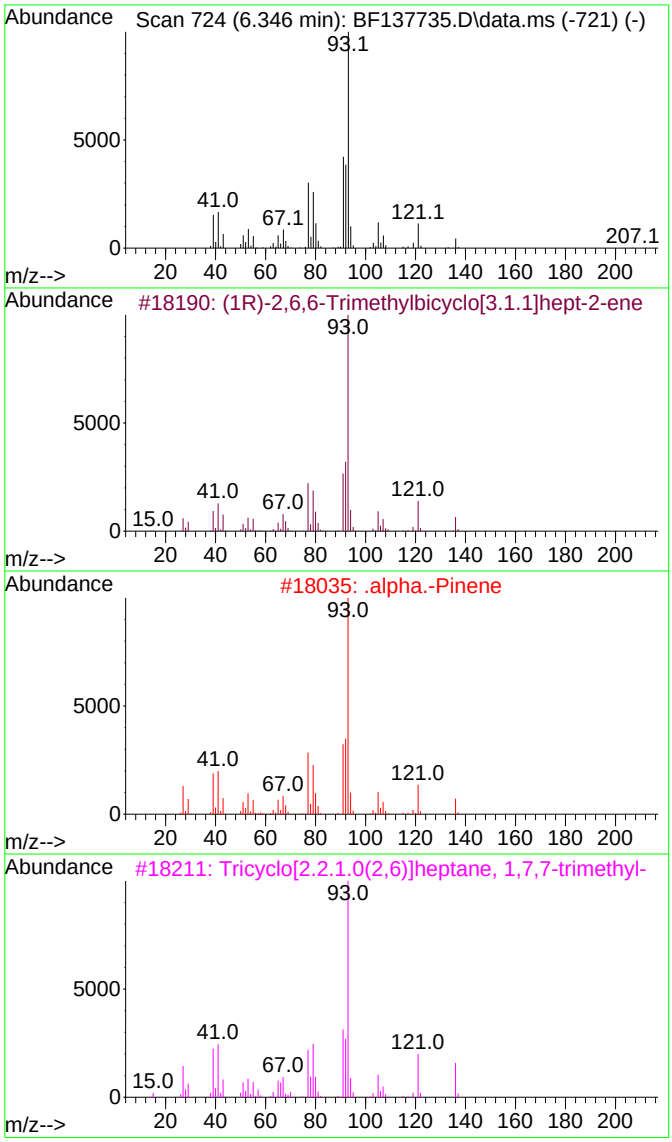
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

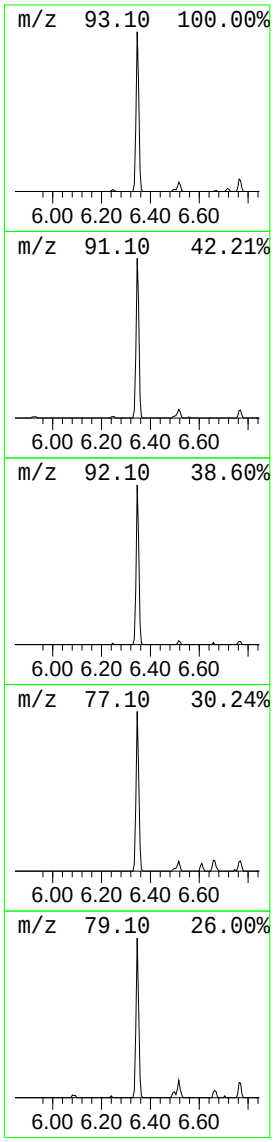
****

Peak Number 3 (1R)-2,6,6-Trimethylbicyclo... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.346	2.32 ng	181631	1,4-Dichlorobenzene-d4	7.057

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(1R)-2,6,6-Trimethylbicyclo[3.1....	136	C10H16	007785-70-8	95
2	.alpha.-Pinene	136	C10H16	000080-56-8	95
3	Tricyclo[2.2.1.0(2,6)]heptane, 1...	136	C10H16	000508-32-7	91
4	Bicyclo[3.1.1]hept-2-ene, 3,6,6-...	136	C10H16	004889-83-2	87
5	(+)-3-Carene	136	C10H16	000498-15-7	87





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF042624\
Data File : BF137735.D
Acq On : 26 Apr 2024 15:16
Operator : CG\JU
Sample : P2218-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
B-131-GW-01

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042324.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

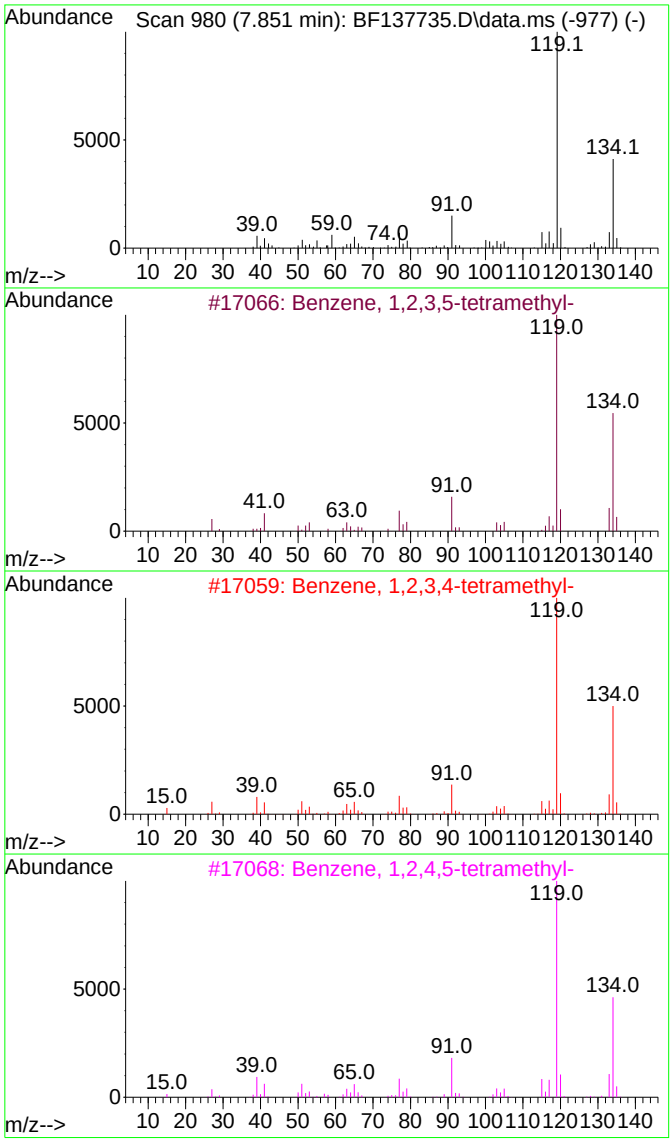
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

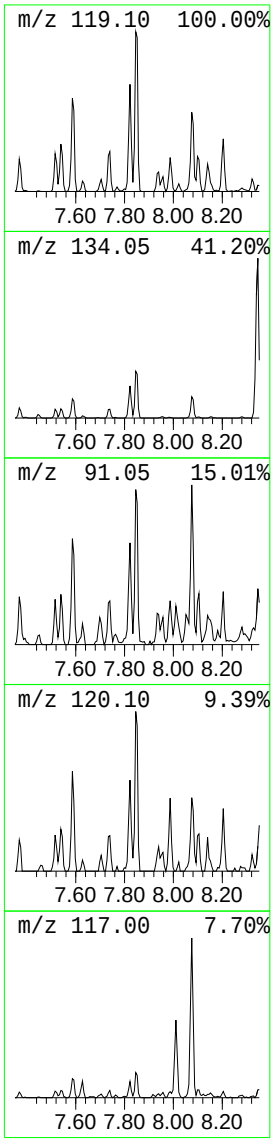
****

Peak Number 4 Benzene, 1,2,3,5-tetramethyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.851	2.09 ng	246308	Naphthalene-d8	8.345

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1,2,3,5-tetramethyl-	134	C10H14	000527-53-7	96
2	Benzene, 1,2,3,4-tetramethyl-	134	C10H14	000488-23-3	95
3	Benzene, 1,2,4,5-tetramethyl-	134	C10H14	000095-93-2	95
4	p-Cymene	134	C10H14	000099-87-6	95
5	o-Cymene	134	C10H14	000527-84-4	94





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF042624\
Data File : BF137735.D
Acq On : 26 Apr 2024 15:16
Operator : CG\JU
Sample : P2218-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
B-131-GW-01

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042324.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

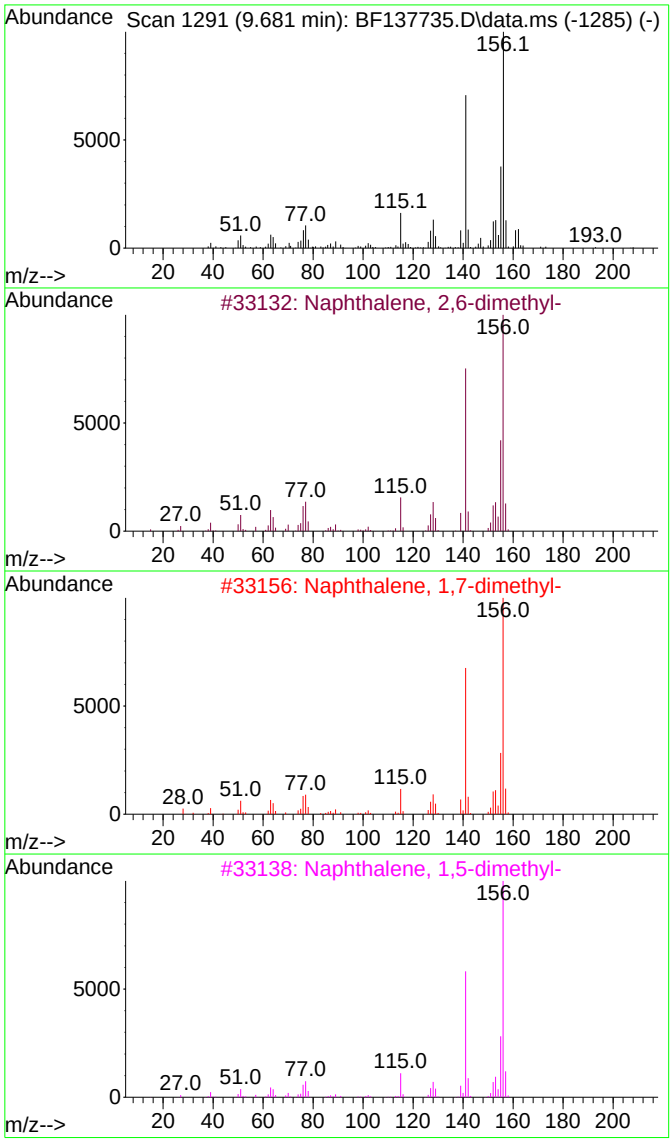
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

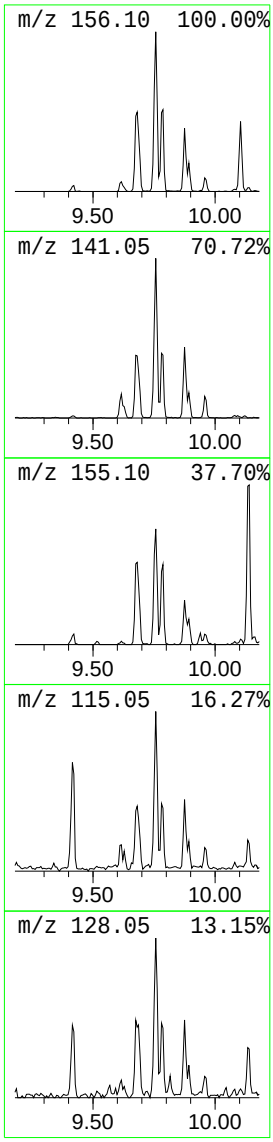
****

Peak Number 5 Naphthalene, 2,6-dimethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.681	2.40 ng	285708	Acenaphthene-d10	10.104

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 2,6-dimethyl-	156	C12H12	000581-42-0	98
2	Naphthalene, 1,7-dimethyl-	156	C12H12	000575-37-1	97
3	Naphthalene, 1,5-dimethyl-	156	C12H12	000571-61-9	97
4	Naphthalene, 1,6-dimethyl-	156	C12H12	000575-43-9	97
5	Naphthalene, 1,2-dimethyl-	156	C12H12	000573-98-8	96





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF042624\
Data File : BF137735.D
Acq On : 26 Apr 2024 15:16
Operator : CG\JU
Sample : P2218-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
B-131-GW-01

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042324.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

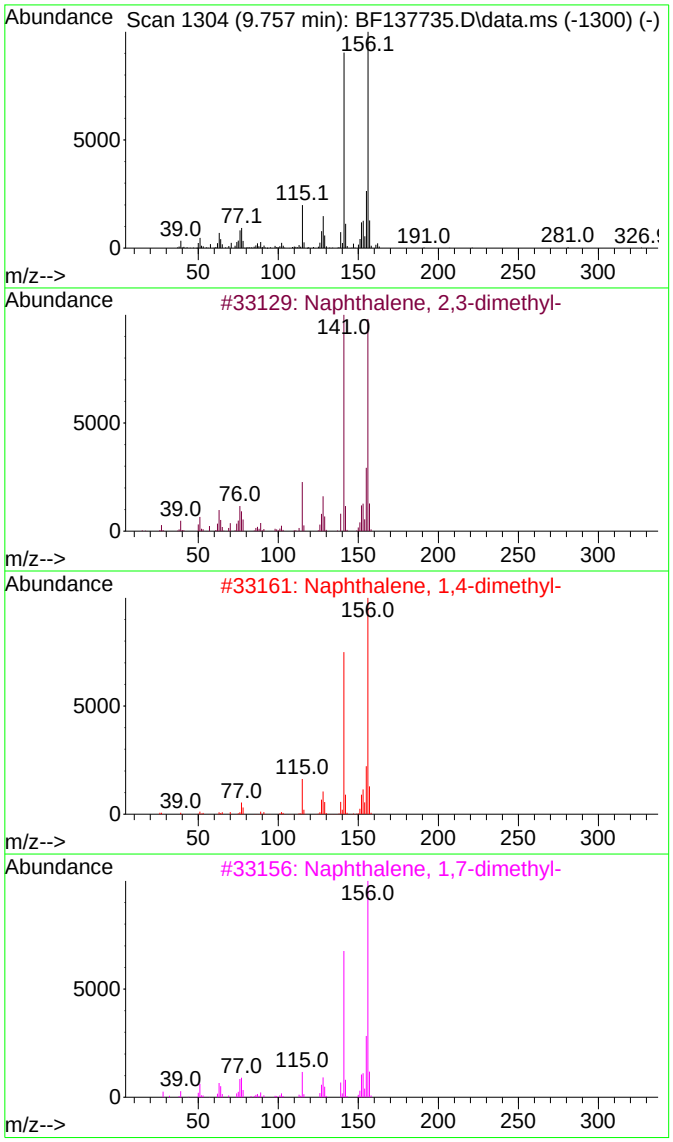
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

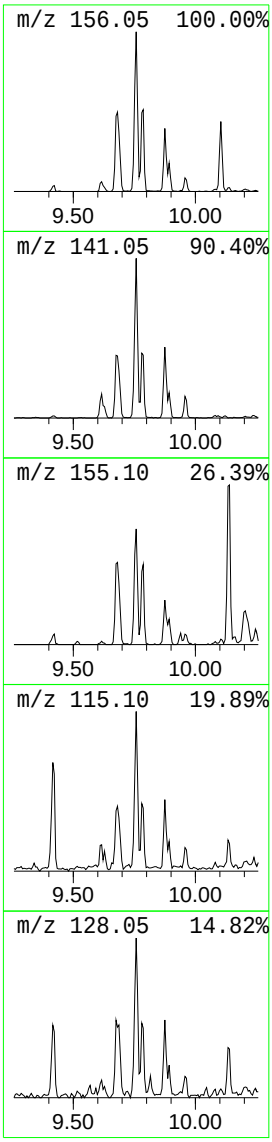
****

Peak Number 6 Naphthalene, 2,3-dimethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.757	3.01 ng	358978	Acenaphthene-d10	10.104

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 2,3-dimethyl-	156	C12H12	000581-40-8	98
2	Naphthalene, 1,4-dimethyl-	156	C12H12	000571-58-4	97
3	Naphthalene, 1,7-dimethyl-	156	C12H12	000575-37-1	97
4	Naphthalene, 1,2-dimethyl-	156	C12H12	000573-98-8	97
5	Naphthalene, 1,3-dimethyl-	156	C12H12	000575-41-7	96





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF042624\
Data File : BF137735.D
Acq On : 26 Apr 2024 15:16
Operator : CG\JU
Sample : P2218-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
B-131-GW-01

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042324.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

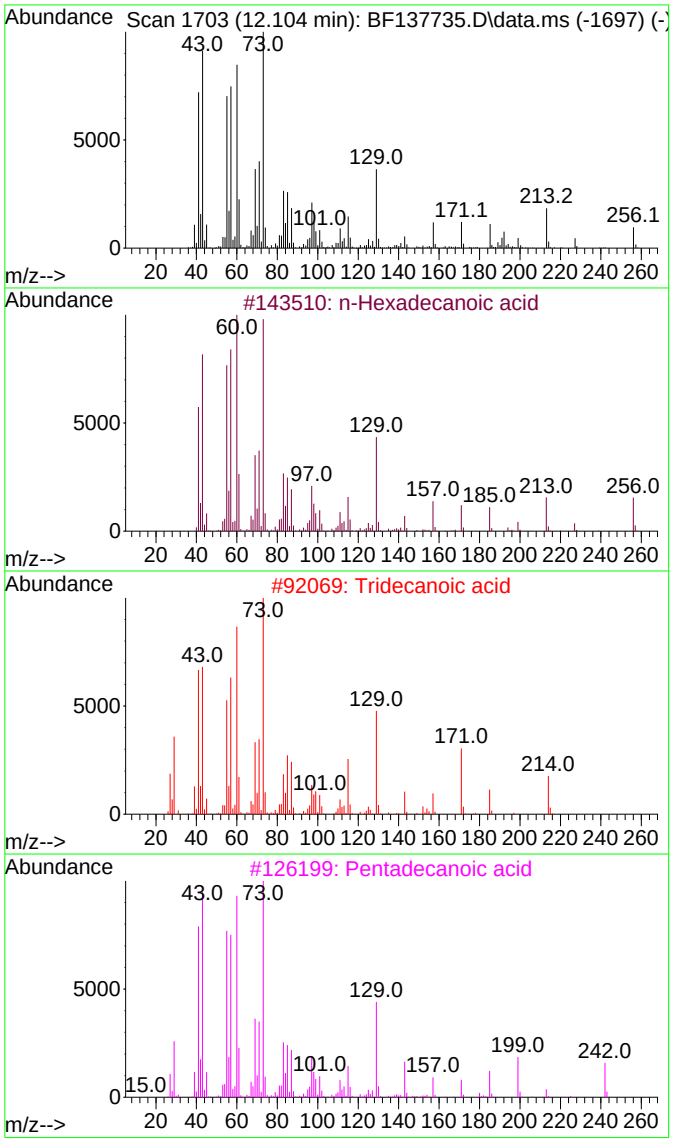
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

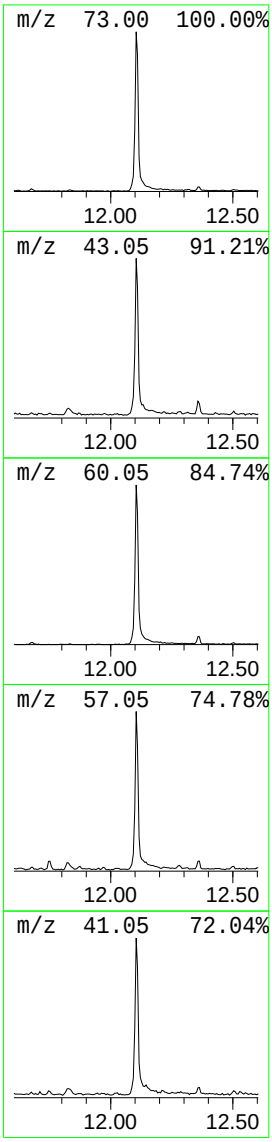
****

Peak Number 7 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.104	8.25 ng	1012560	Phenanthrene-d10	11.598

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	95
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	93
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	91
5	8-Methylnonanoic acid	172	C10H20O2	005963-14-4	58





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF042624\
Data File : BF137735.D
Acq On : 26 Apr 2024 15:16
Operator : CG\JU
Sample : P2218-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
B-131-GW-01

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042324.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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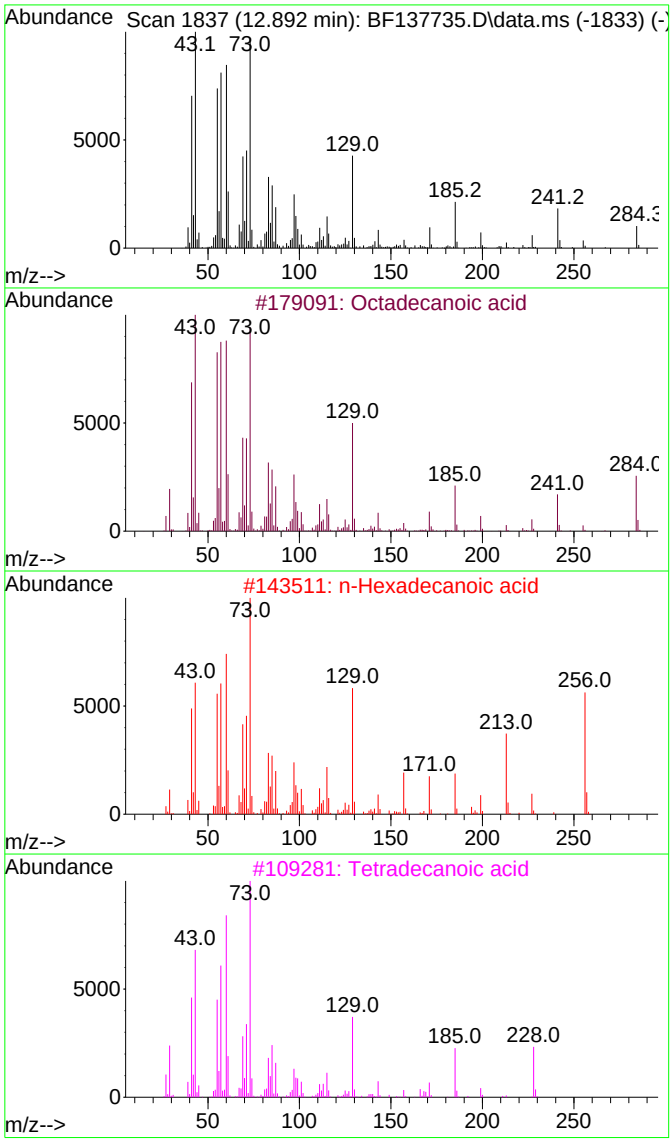
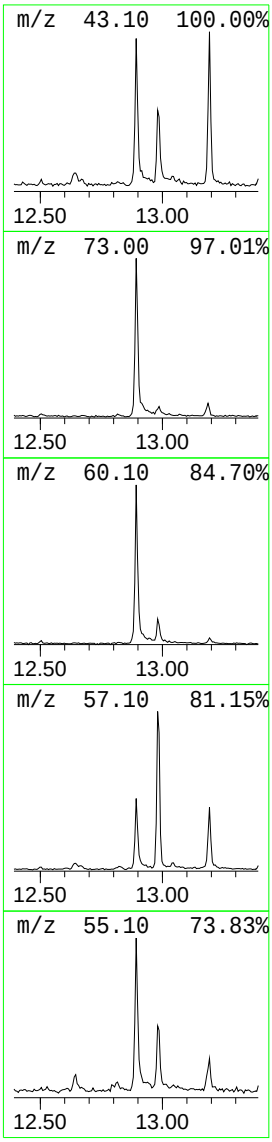
Peak Number 8 Octadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.892	3.69 ng	453353	Phenanthrene-d10	11.598

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	91
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	90
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	76
5	n-Decanoic acid	172	C10H20O2	000334-48-5	70





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF042624\
Data File : BF137735.D
Acq On : 26 Apr 2024 15:16
Operator : CG\JU
Sample : P2218-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
B-131-GW-01

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042324.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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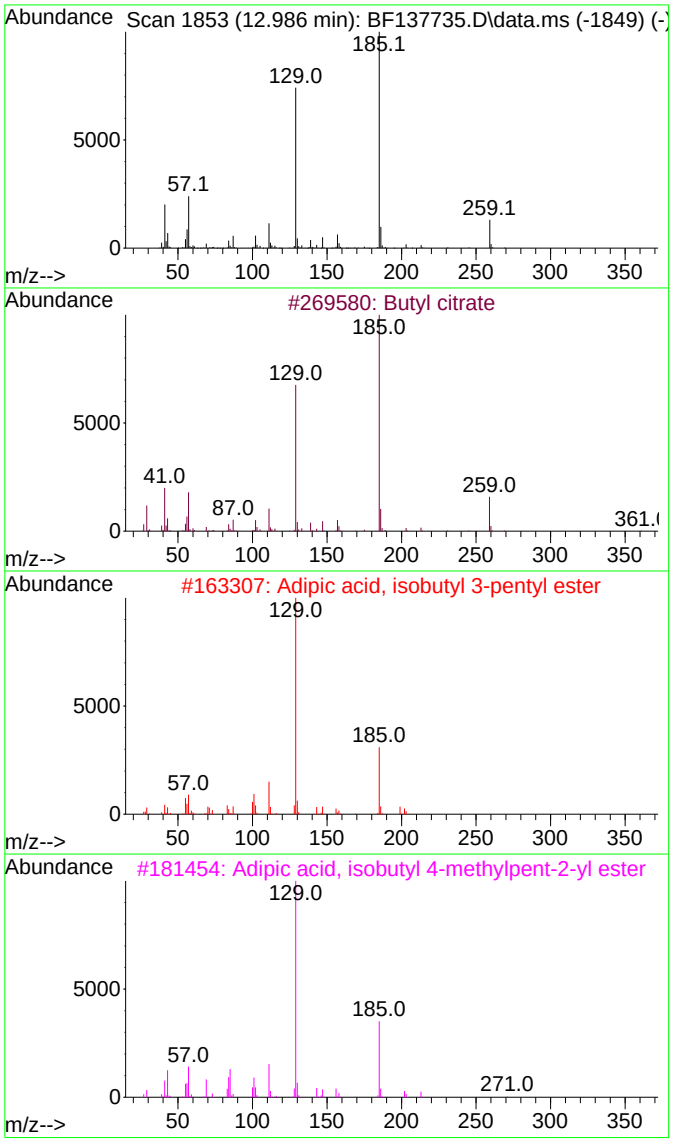
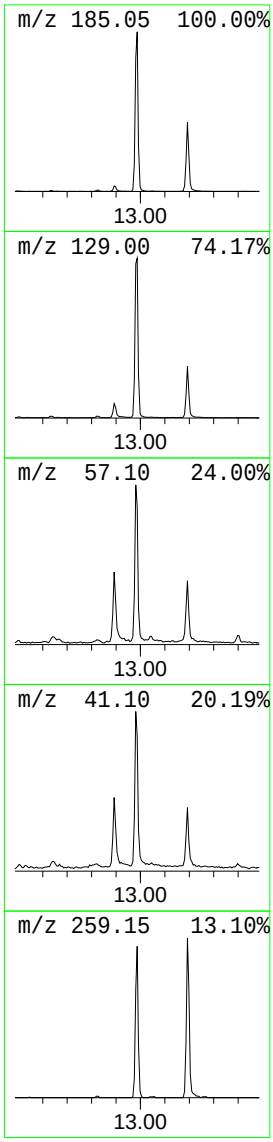
Peak Number 9 Butyl citrate Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.986	12.38 ng	844002	Chrysene-d12	14.245

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butyl citrate	360	C18H32O7	000077-94-1	91
2	Adipic acid, isobutyl 3-pentyl e...	272	C15H28O4	1000324-60-4	78
3	Adipic acid, isobutyl 4-methylpe...	286	C16H30O4	1000353-50-1	64
4	Hexanedioic acid, bis(2-methylpr...	258	C14H26O4	000141-04-8	64
5	Adipic acid, 2,4-dimethylpent-3-...	300	C17H32O4	1000349-77-6	64





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF042624\
Data File : BF137735.D
Acq On : 26 Apr 2024 15:16
Operator : CG\JU
Sample : P2218-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
B-131-GW-01

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042324.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

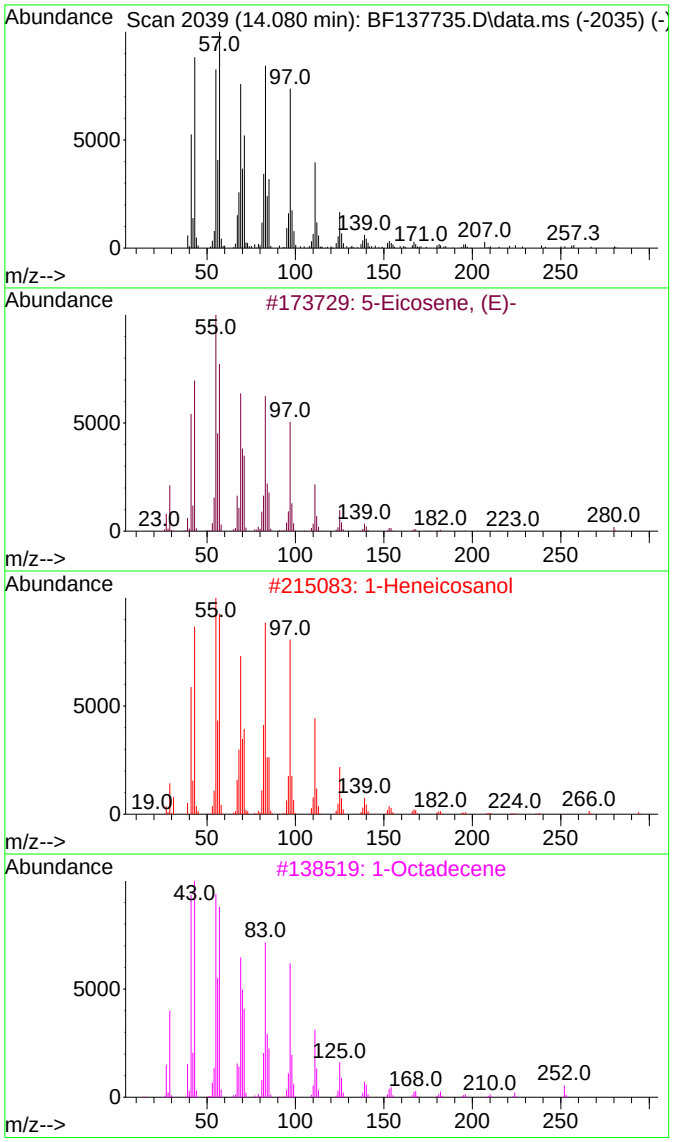
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

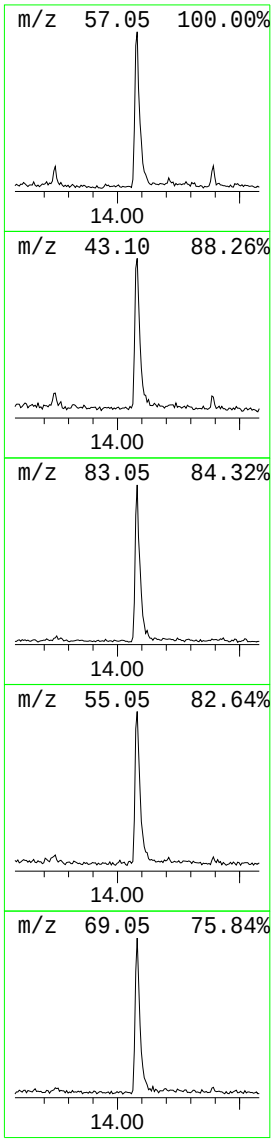
****

Peak Number 10 5-Eicosene, (E)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.080	6.53 ng	445540	Chrysene-d12	14.245

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Eicosene, (E)-	280	C20H40	074685-30-6	98
2	1-Heneicosanol	312	C21H44O	015594-90-8	95
3	1-Octadecene	252	C18H36	000112-88-9	94
4	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	94
5	Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	94





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF042624\
Data File : BF137735.D
Acq On : 26 Apr 2024 15:16
Operator : CG\JU
Sample : P2218-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
B-131-GW-01

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042324.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...	2.434	18.5	ng	1443850	1	7.057	1562670	20.0
(1R)-2,6,6-Trim...	6.346	2.3	ng	181631	1	7.057	1562670	20.0
Benzene, 1,2,3,...	7.851	2.1	ng	246308	2	8.345	2353200	20.0
Naphthalene, 2,...	9.681	2.4	ng	285708	3	10.104	2383910	20.0
Naphthalene, 2,...	9.757	3.0	ng	358978	3	10.104	2383910	20.0
n-Hexadecanoic ...	12.104	8.3	ng	1012560	4	11.598	2456120	20.0
Octadecanoic acid	12.892	3.7	ng	453353	4	11.598	2456120	20.0
Butyl citrate	12.986	12.4	ng	844002	5	14.245	1363950	20.0
5-Eicosene, (E)-	14.080	6.5	ng	445540	5	14.245	1363950	20.0