LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111022\
Data File : BF131140.D
Acq On : 11 Nov 2022 00:15
Operator : CG\JU
Sample : N5491-10
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-4

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-BF110922.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF131140.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.152	5	11	19	rVB	492070	628611	43.94%	5.680%
2	2.263	26	30	37	rVB	24742	32814	2.29%	0.297%
3	4.487	404	408	413	rBV	38834	45561	3.18%	0.412%
4	5.104	509	513	523	rBV	289888	353979	24.74%	3.199%
5	5.504	577	581	585	rBV	1432434	1430511	100.00%	12.926%
6	6.516	748	753	756	rBV	1496973	1380166	96.48%	12.471%
7	6.887	813	816	820	rBV	505470	404335	28.27%	3.654%
8	7.451	908	912	915	rBV	1034378	923413	64.55%	8.344%
9	8.175	1031	1035	1038	rBV	510521	443720	31.02%	4.009%
10	9.245	1213	1217	1221	rBV	1435322	1293349	90.41%	11.687%
11	9.933	1330	1334	1337	rBV	555081	464220	32.45%	4.195%
12	10.722	1464	1468	1476	rBV	886346	750744	52.48%	6.784%
13	11.422	1584	1587	1591	rBV	479016	416911	29.14%	3.767%
14	12.639	1791	1794	1799	rBV	22102	18366	1.28%	0.166%
15	12.869	1831	1833	1836	rVB	17237	15227	1.06%	0.138%
16	13.010	1853	1857	1861	rBV	1324614	1224890	85.63%	11.068%
17	13.968	2014	2020	2031	rBV5	69928	248233	17.35%	2.243%
18	14.074	2034	2038	2041	rBV	525914	472477	33.03%	4.269%
19	14.168	2050	2054	2058	rVV	78627	83042	5.81%	0.750%
20	14.221	2061	2063	2071	rVB4	19398	29350	2.05%	0.265%
21	14.527	2113	2115	2120	rVB3	29239	34236	2.39%	0.309%
22	14.921	2179	2182	2185	rVB	37045	34518	2.41%	0.312%
23	15.192	2225	2228	2231	rVB3	14923	16341	1.14%	0.148%
24	15.268	2239	2241	2245	rBV4	11481	16831	1.18%	0.152%
25	15.568	2288	2292	2300	rVB	228417	305069	21.33%	2.757%

Sum of corrected areas: 11066914

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111022\
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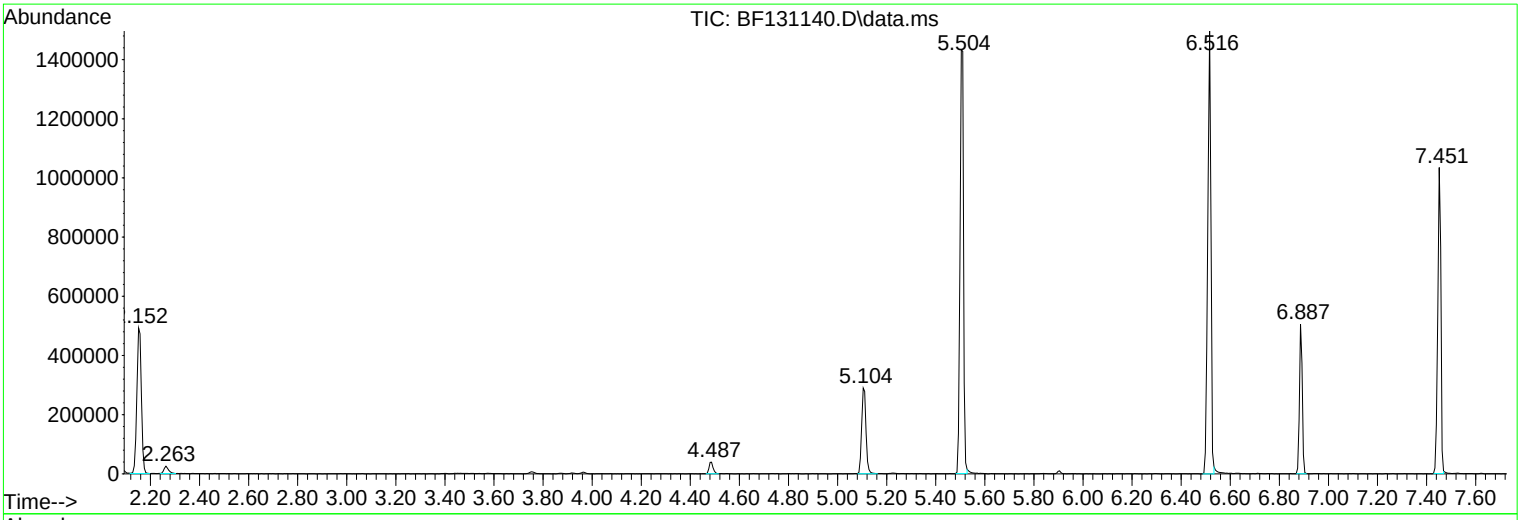
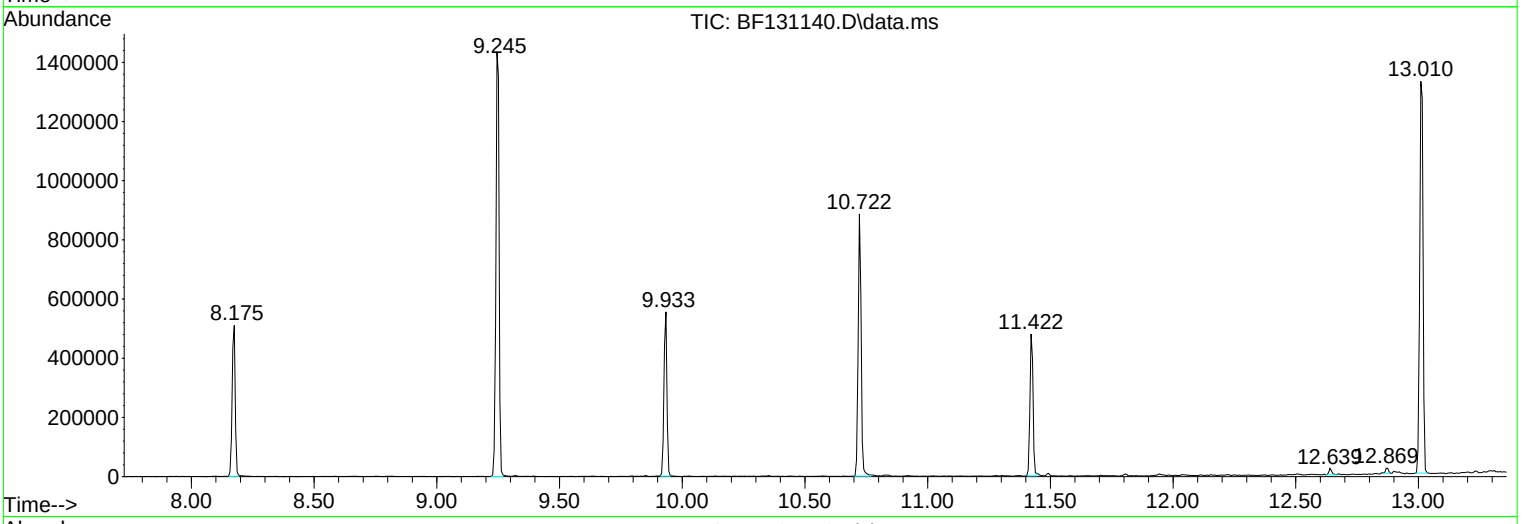
Misc :
ALS Vial : 17 Sample Multiplier: 1

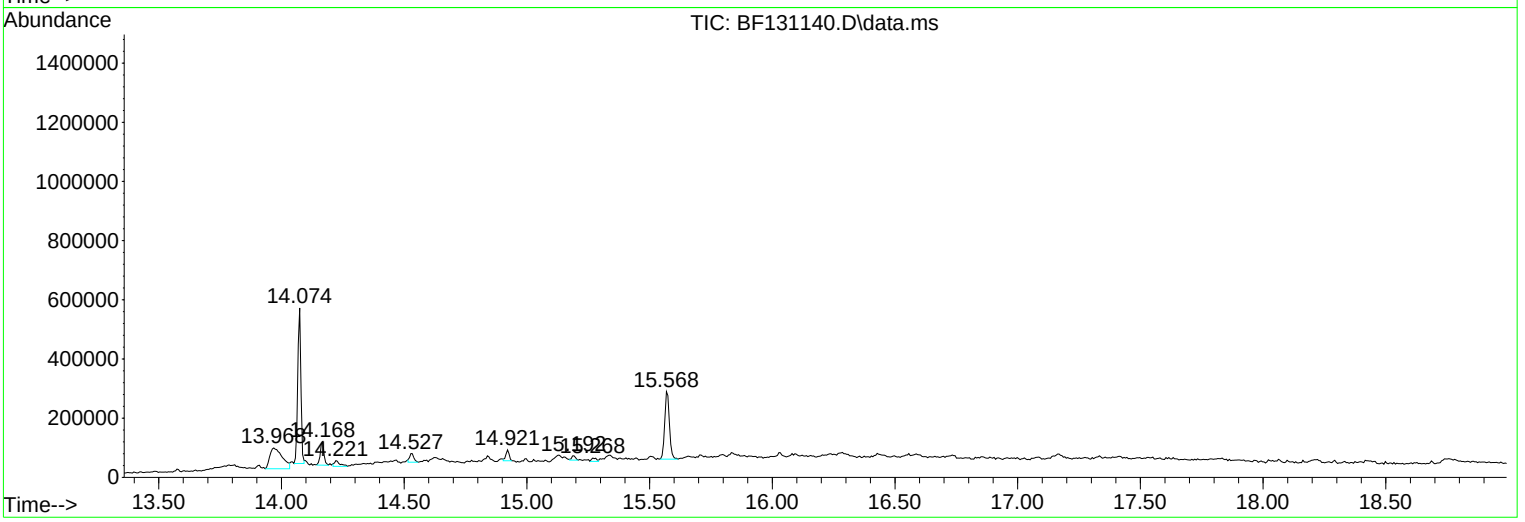
Instrument :
BNA_F
ClientSampleId :
TP-4

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF110922.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\BF111022\
Data File : BF131140.D
Acq On : 11 Nov 2022 00:15
Operator : CG\JU
Sample : N5491-10
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF110922.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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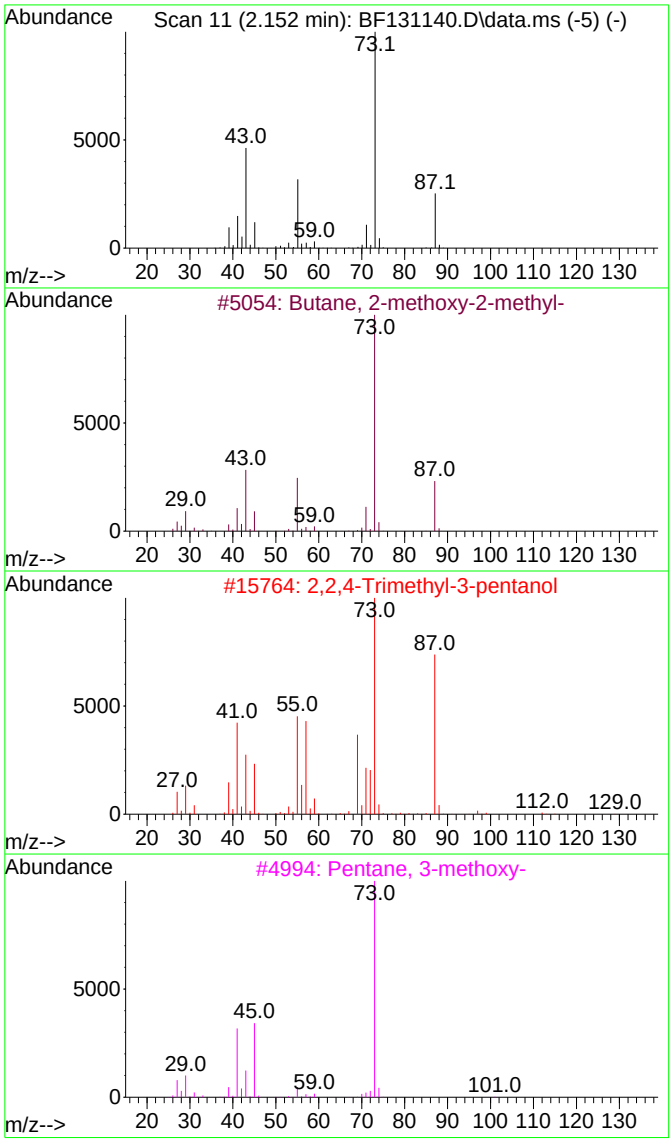
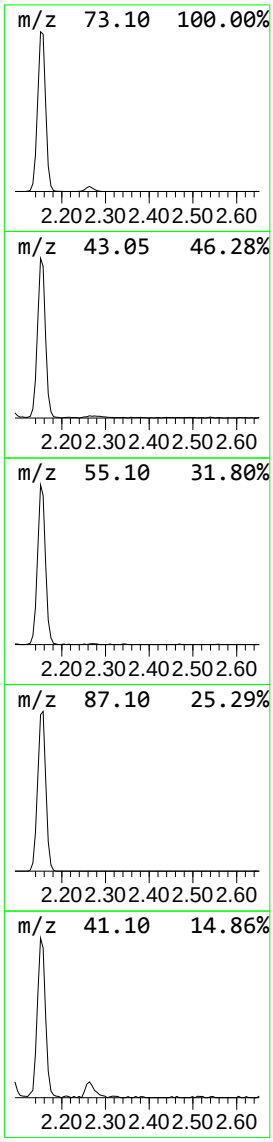
Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.152	31.09 ng	628611	1,4-Dichlorobenzene-d4	6.887

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	39
3	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12
4	Silane, tetramethyl-	88	C4H12Si	000075-76-3	12
5	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111022\
Data File : BF131140.D
Acq On : 11 Nov 2022 00:15
Operator : CG\JU
Sample : N5491-10
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-4

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF110922.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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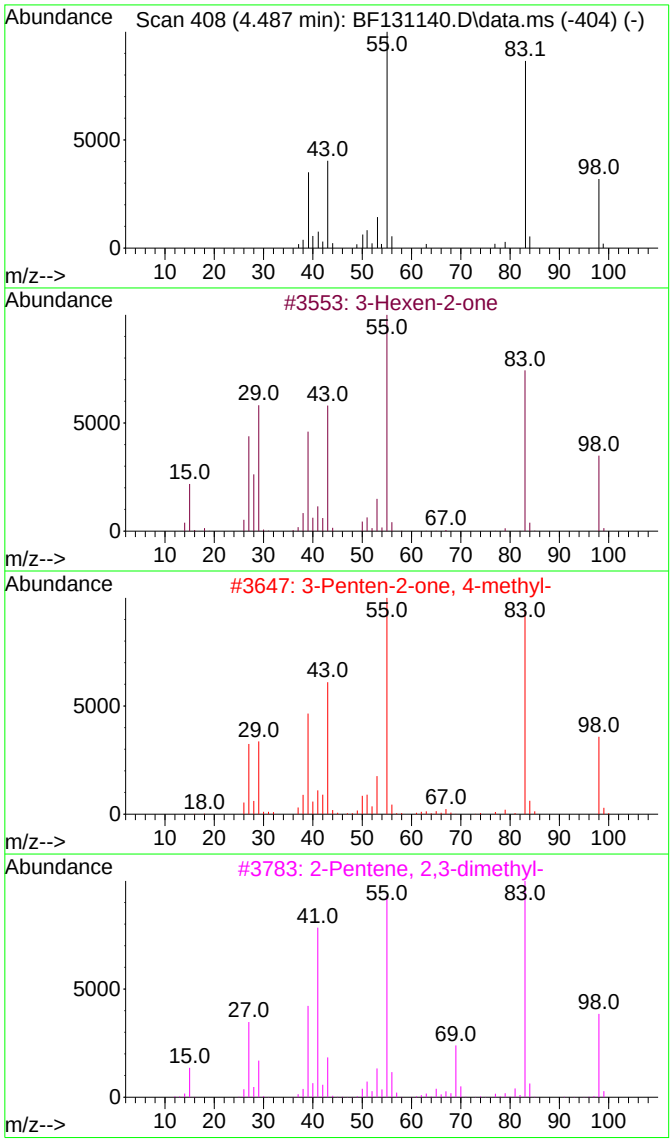
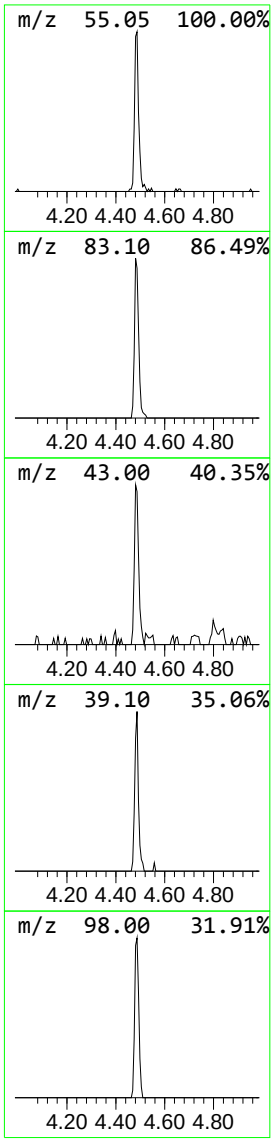
Peak Number 2 3-Hexen-2-one Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.487	2.25 ng	45561	1,4-Dichlorobenzene-d4	6.887

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Hexen-2-one	98	C6H10O	000763-93-9	91
2	3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	90
3	2-Pentene, 2,3-dimethyl-	98	C7H14	010574-37-5	80
4	2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	78
5	2-Pentene, 4,4-dimethyl-, (E)-	98	C7H14	000690-08-4	78





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111022\
Data File : BF131140.D
Acq On : 11 Nov 2022 00:15
Operator : CG\JU
Sample : N5491-10
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-4

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF110922.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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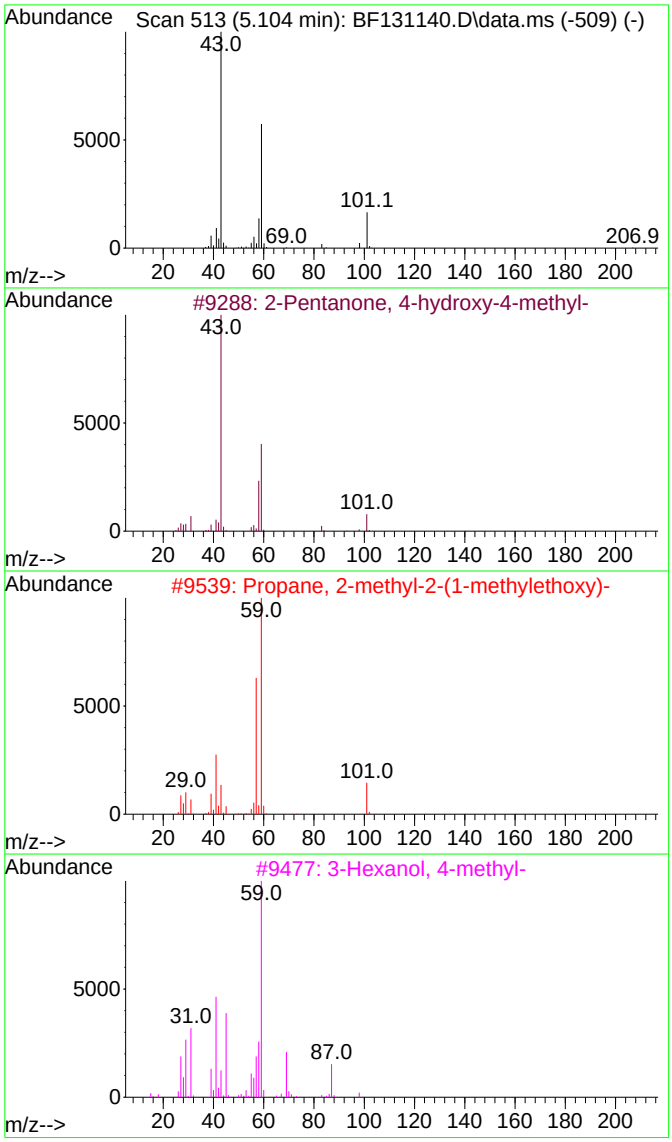
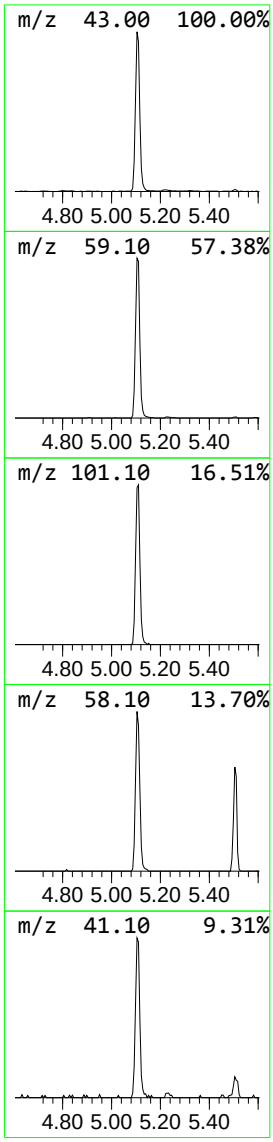
Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.104	17.51 ng	353979	1,4-Dichlorobenzene-d4	6.887

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	42
3	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
5	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111022\
Data File : BF131140.D
Acq On : 11 Nov 2022 00:15
Operator : CG\JU
Sample : N5491-10
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-4

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF110922.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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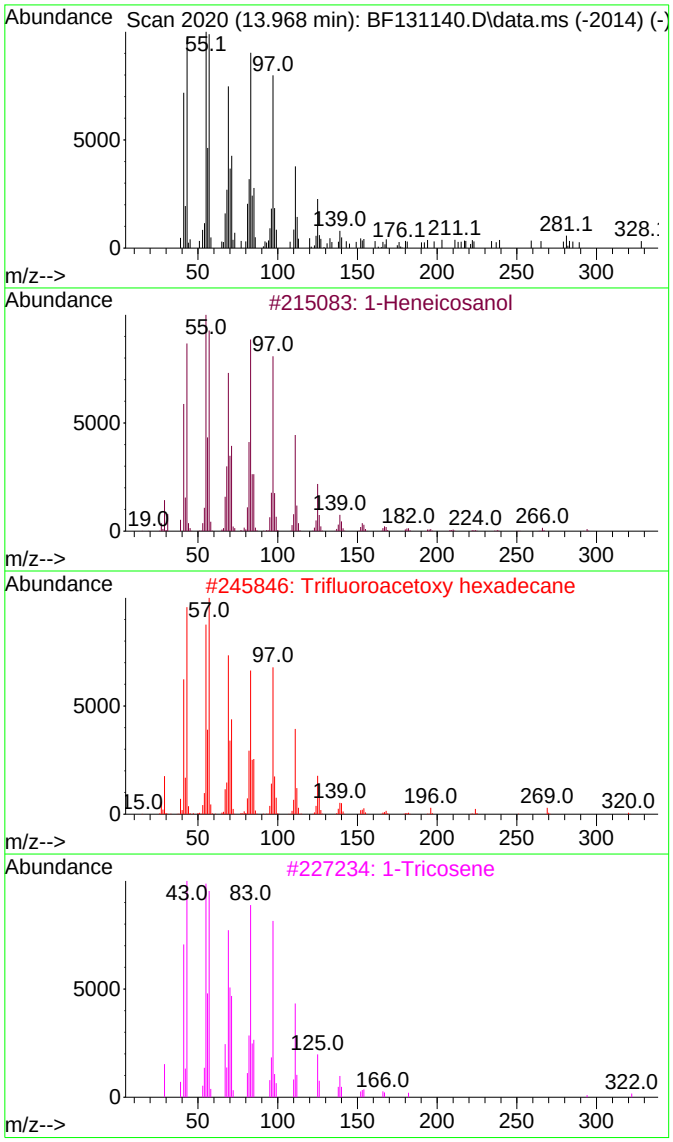
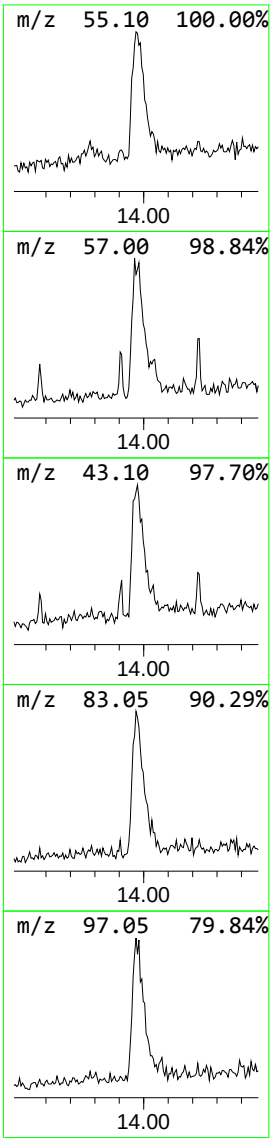
Peak Number 4 1-Heneicosanol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.969	10.51 ng	248233	Chrysene-d12	14.074

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol	312	C21H44O	015594-90-8	95
2	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	94
3	1-Tricosene	322	C23H46	018835-32-0	94
4	n-Tetracosanol-1	354	C24H50O	000506-51-4	93
5	1-Heptacosanol	396	C27H56O	002004-39-9	93





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111022\
Data File : BF131140.D
Acq On : 11 Nov 2022 00:15
Operator : CG\JU
Sample : N5491-10
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-4

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF110922.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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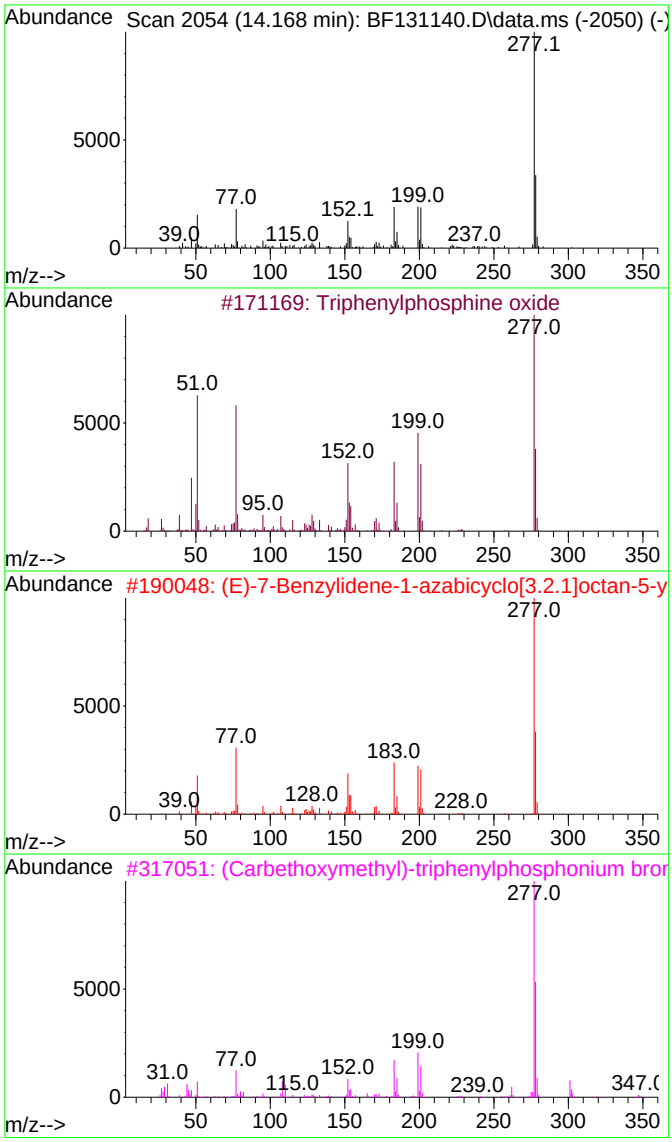
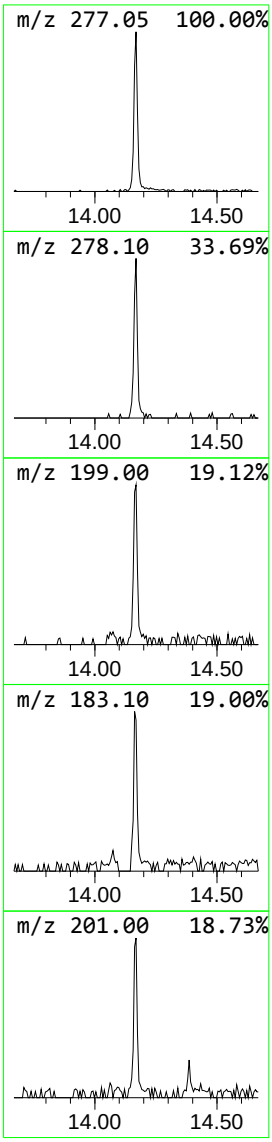
Peak Number 5 Triphenylphosphine oxide Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.169	3.52 ng	83042	Chrysene-d12	14.074

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Triphenylphosphine oxide	278	C18H15OP	000791-28-6	97
2	(E)-7-Benzylidene-1-azabicyclo[3...	293	C15H19NO3S	1000483-83-4	58
3	(Carbethoxymethyl)-triphenylphos...	428	C22H22BrO2P	001530-45-6	45
4	Formaldehyde, (triphenylphosphor...	304	C19H17N2P	015990-54-2	37
5	5-Methyl-8-phenylfuro[3',2':5,6]...	277	C16H11N3O2	1000460-07-9	28





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111022\
Data File : BF131140.D
Acq On : 11 Nov 2022 00:15
Operator : CG\JU
Sample : N5491-10
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-4

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF110922.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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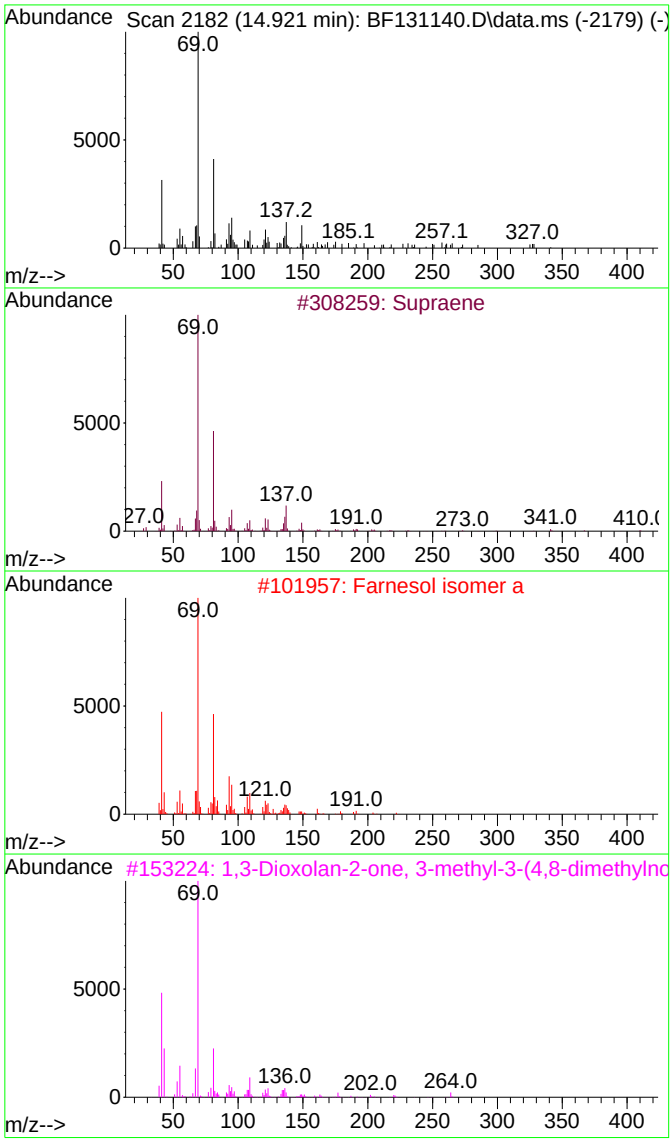
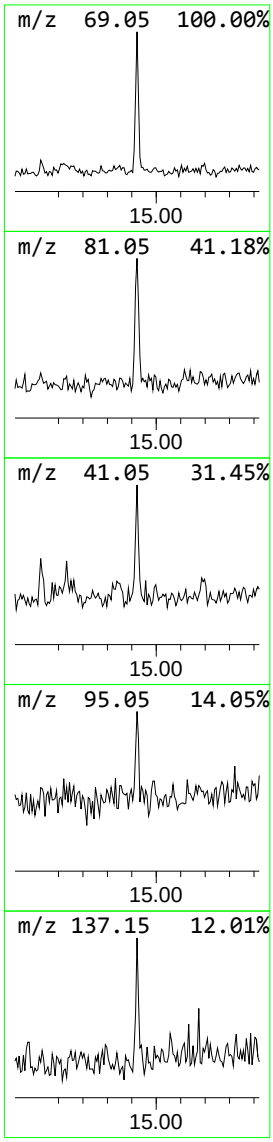
Peak Number 6 Supraene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.921	2.26 ng	34518	Perylene-d12	15.568

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Supraene	410	C30H50	007683-64-9	74
2	Farnesol isomer a	222	C15H26O	1000108-92-4	59
3	1,3-Dioxolan-2-one, 3-methyl-3-(...	264	C16H24O3	336879-76-6	58
4	2,6-Octadiene, 4-methyl-	124	C9H16	074498-94-5	53
5	trans-Farnesol	222	C15H26O	000106-28-5	53





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111022\
Data File : BF131140.D
Acq On : 11 Nov 2022 00:15
Operator : CG\JU
Sample : N5491-10
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-4

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF110922.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...	2.152	31.1	ng	628611	1	6.887	404335	20.0
3-Hexen-2-one	4.487	2.3	ng	45561	1	6.887	404335	20.0
2-Pentanone, 4-...	5.104	17.5	ng	353979	1	6.887	404335	20.0
1-Heneicosanol	13.969	10.5	ng	248233	5	14.074	472477	20.0
Triphenylphosph...	14.169	3.5	ng	83042	5	14.074	472477	20.0
Supraene	14.921	2.3	ng	34518	6	15.568	305069	20.0