LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122721\
Data File : BF126375.D
Acq On : 28 Dec 2021 1:20
Operator : JU/CG
Sample : M5235-01 5X
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
HD-02-122321

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-BF121521.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF126375.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.369	384	388	396	rBV	57759	67325	7.57%	0.755%
2	4.998	491	495	507	rVB	176403	181280	20.38%	2.034%
3	5.410	562	565	579	rVB	414016	421758	47.41%	4.733%
4	5.822	631	635	641	rVB	12925	12173	1.37%	0.137%
5	6.434	735	739	757	rVB	407755	405904	45.63%	4.555%
6	6.810	799	803	806	rBV	638261	500818	56.30%	5.620%
7	7.369	894	898	904	rBV	250897	236673	26.60%	2.656%
8	7.416	904	906	909	rVB	16628	13875	1.56%	0.156%
9	8.092	1016	1021	1028	rBV	705180	602964	67.78%	6.766%
10	8.163	1028	1033	1035	rVB	18483	22733	2.56%	0.255%
11	8.392	1064	1072	1074	rBV4	9513	16714	1.88%	0.188%
12	8.522	1091	1094	1096	rBV	24885	18598	2.09%	0.209%
13	8.692	1119	1123	1126	rBV	31981	26315	2.96%	0.295%
14	8.975	1168	1171	1175	rBV3	7438	11789	1.33%	0.132%
15	9.122	1193	1196	1200	rVB2	21870	18531	2.08%	0.208%
16	9.169	1200	1204	1209	rBV	428063	355986	40.02%	3.995%
17	9.257	1216	1219	1224	rBV	40866	36089	4.06%	0.405%
18	9.575	1268	1273	1275	rBV2	24616	30682	3.45%	0.344%
19	9.786	1307	1309	1314	rVB	33579	25936	2.92%	0.291%
20	9.845	1316	1319	1326	rVB	602753	521854	58.66%	5.856%
21	10.263	1387	1390	1392	rBV2	13310	14054	1.58%	0.158%
22	10.286	1392	1394	1397	rVB	29016	23059	2.59%	0.259%
23	10.504	1427	1431	1434	rBV	14494	16003	1.80%	0.180%
24	10.633	1449	1453	1457	rBV	203337	182889	20.56%	2.052%
25	10.757	1471	1474	1483	rBV2	33074	47661	5.36%	0.535%
26	10.863	1488	1492	1496	rBV4	14131	14238	1.60%	0.160%
27	11.204	1547	1550	1553	rBV2	24133	21689	2.44%	0.243%
28	11.239	1553	1556	1561	rVB3	15875	15834	1.78%	0.178%
29	11.333	1568	1572	1575	rBV	615200	536538	60.31%	6.021%
30	11.633	1620	1623	1625	rBV	24185	20067	2.26%	0.225%
31	11.657	1625	1627	1630	rVB2	67519	49417	5.55%	0.555%
32	11.733	1636	1640	1647	rVB	653250	503837	56.64%	5.654%
33	11.863	1660	1662	1666	rBV3	14131	13975	1.57%	0.157%
34	11.945	1674	1676	1686	rVB10	9439	16911	1.90%	0.190%
35	12.039	1690	1692	1695	rBV	24002	19514	2.19%	0.219%
36	12.321	1735	1740	1744	rBV5	9071	17726	1.99%	0.199%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122721\
Data File : BF126375.D
Acq On : 28 Dec 2021 1:20
Operator : JU/CG
Sample : M5235-01 5X
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
HD-02-122321

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-BF121521.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	12.386	1748	1751	1753	rBV3	12674	11968	1.35%	0.134%
38	12.421	1753	1757	1758	rBV	1001429	889608	100.00%	9.982%
39	12.439	1758	1760	1763	rVB	1107880	853090	95.90%	9.573%
40	12.527	1771	1775	1781	rBV2	246306	236899	26.63%	2.658%
41	12.704	1802	1805	1809	rBV6	12352	18750	2.11%	0.210%
42	12.774	1813	1817	1819	rVV	40274	51834	5.83%	0.582%
43	12.798	1819	1821	1825	rVB2	24190	25233	2.84%	0.283%
44	12.915	1838	1841	1847	rBV	476712	441031	49.58%	4.949%
45	13.086	1867	1870	1871	rBV3	18588	17720	1.99%	0.199%
46	13.157	1879	1882	1887	rBV5	42477	60714	6.82%	0.681%
47	13.251	1896	1898	1900	rVB3	17736	13915	1.56%	0.156%
48	13.368	1914	1918	1920	rBV5	24743	31737	3.57%	0.356%
49	13.468	1933	1935	1936	rBV	21824	16159	1.82%	0.181%
50	13.504	1938	1941	1943	rVV2	36051	32984	3.71%	0.370%
51	13.827	1994	1996	1999	rBV	35134	40530	4.56%	0.455%
52	13.974	2017	2021	2024	rBV	605480	603526	67.84%	6.772%
53	14.145	2048	2050	2054	rVB	45627	39759	4.47%	0.446%
54	14.451	2100	2102	2106	rBV	59299	57547	6.47%	0.646%
55	15.421	2263	2267	2271	rBV	353816	427328	48.04%	4.795%

Sum of corrected areas: 8911741

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Acq On : 28 Dec 2021 1:20
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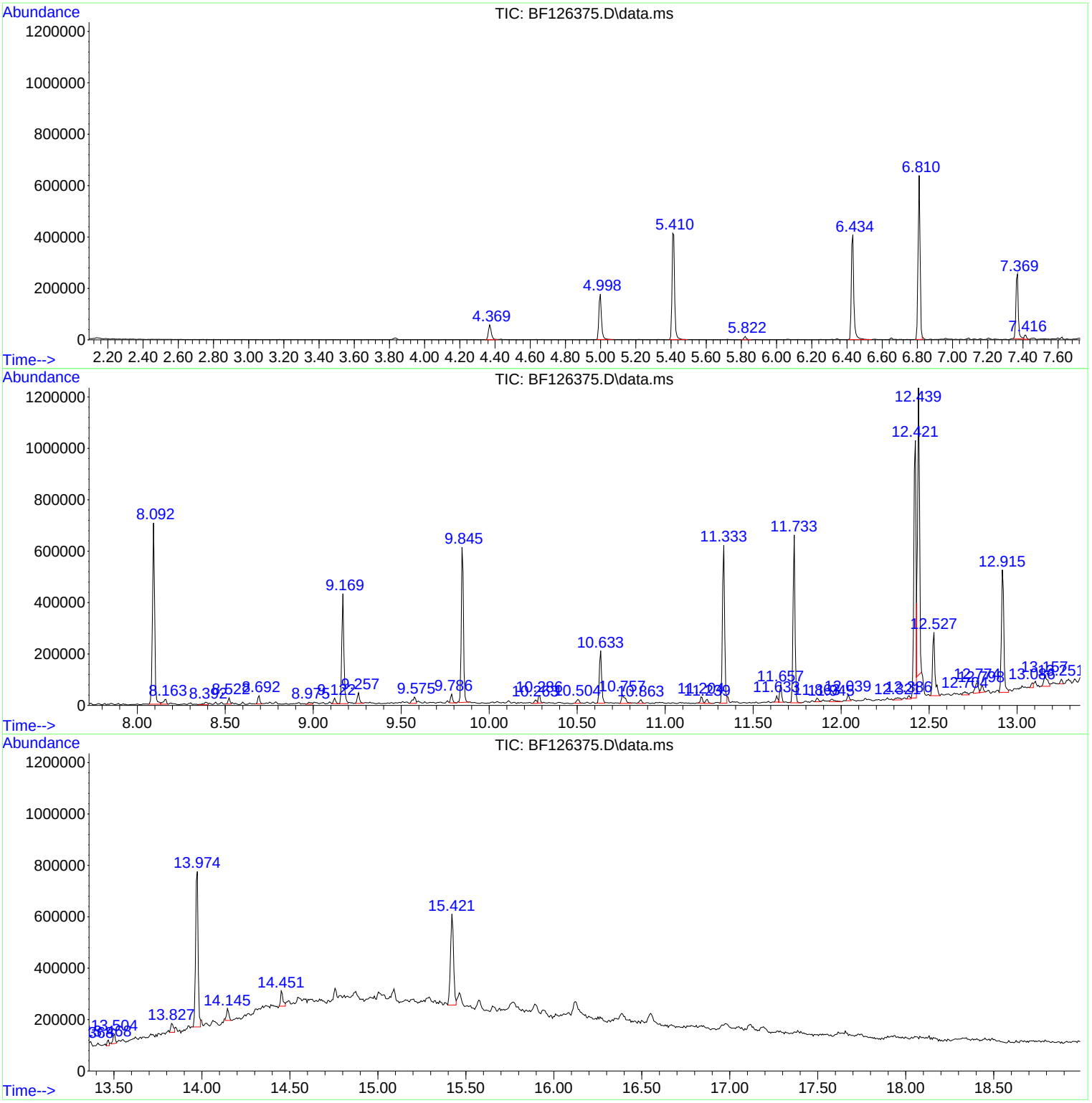
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
HD-02-122321

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF121521.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\BF122721\
Data File : BF126375.D
Acq On : 28 Dec 2021 1:20
Operator : JU/CG
Sample : M5235-01 5X
Misc :
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Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF121521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

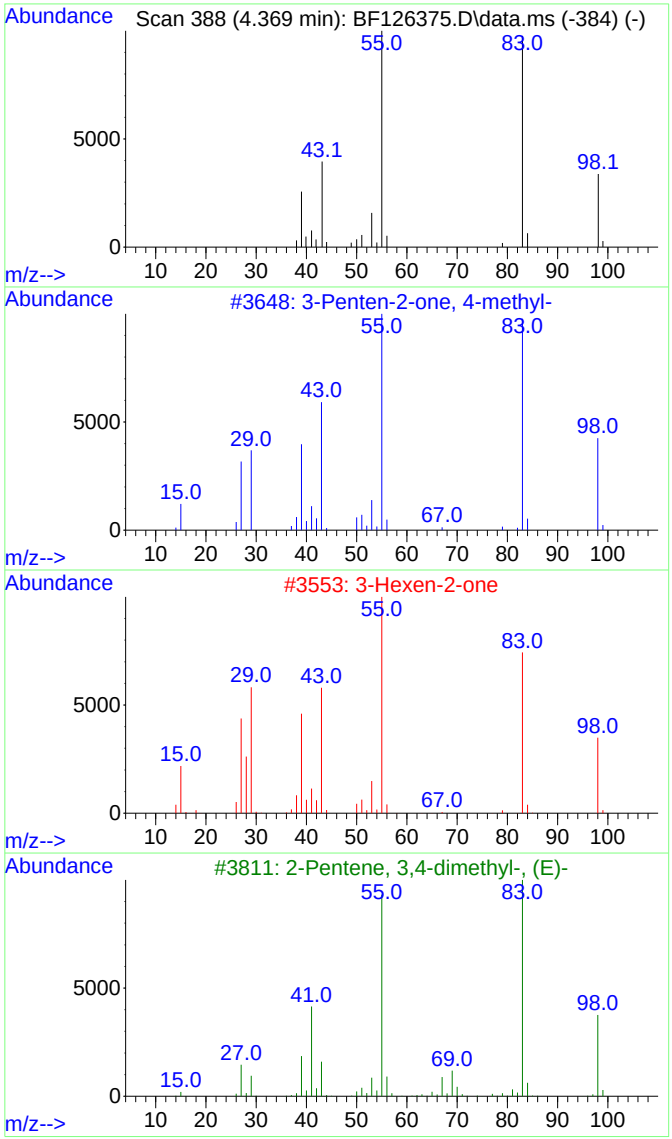
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

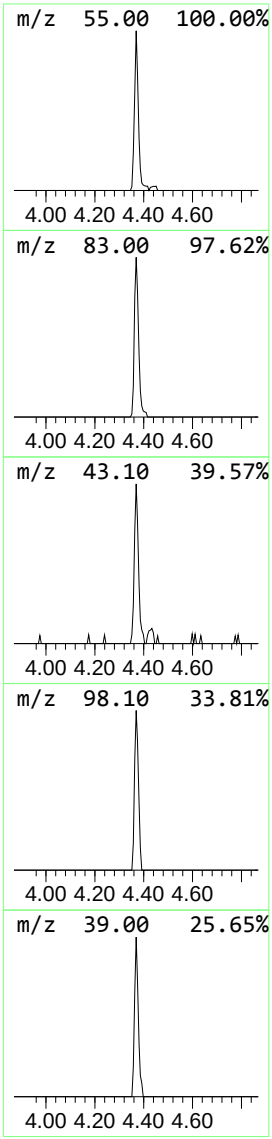
****

Peak Number 1 3-Penten-2-one, 4-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.369	2.69 ng	67325	1,4-Dichlorobenzene-d4	6.810

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	91
2	3-Hexen-2-one	98	C6H10O	000763-93-9	91
3	2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	86
4	2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	86
5	2-Pentene, 4,4-dimethyl-, (E)-	98	C7H14	000690-08-4	86





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122721\
Data File : BF126375.D
Acq On : 28 Dec 2021 1:20
Operator : JU/CG
Sample : M5235-01 5X
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
HD-02-122321

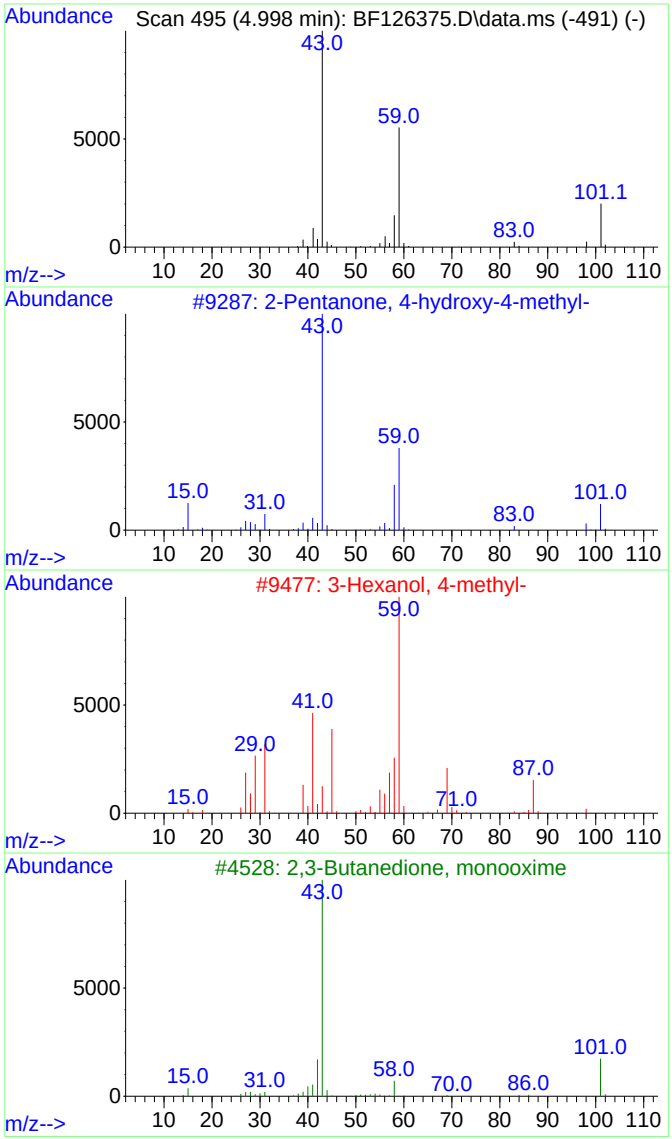
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF121521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

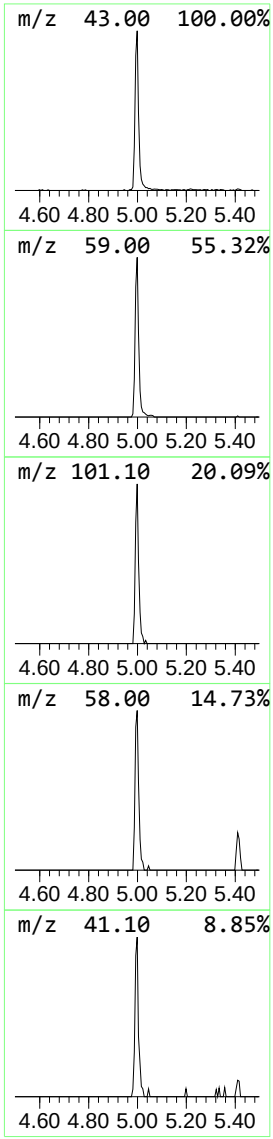
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.998	7.24 ng	181280	1,4-Dichlorobenzene-d4	6.810

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	28
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5	1,2-Butanediol	90	C4H10O2	000584-03-2	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122721\
Data File : BF126375.D
Acq On : 28 Dec 2021 1:20
Operator : JU/CG
Sample : M5235-01 5X
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
HD-02-122321

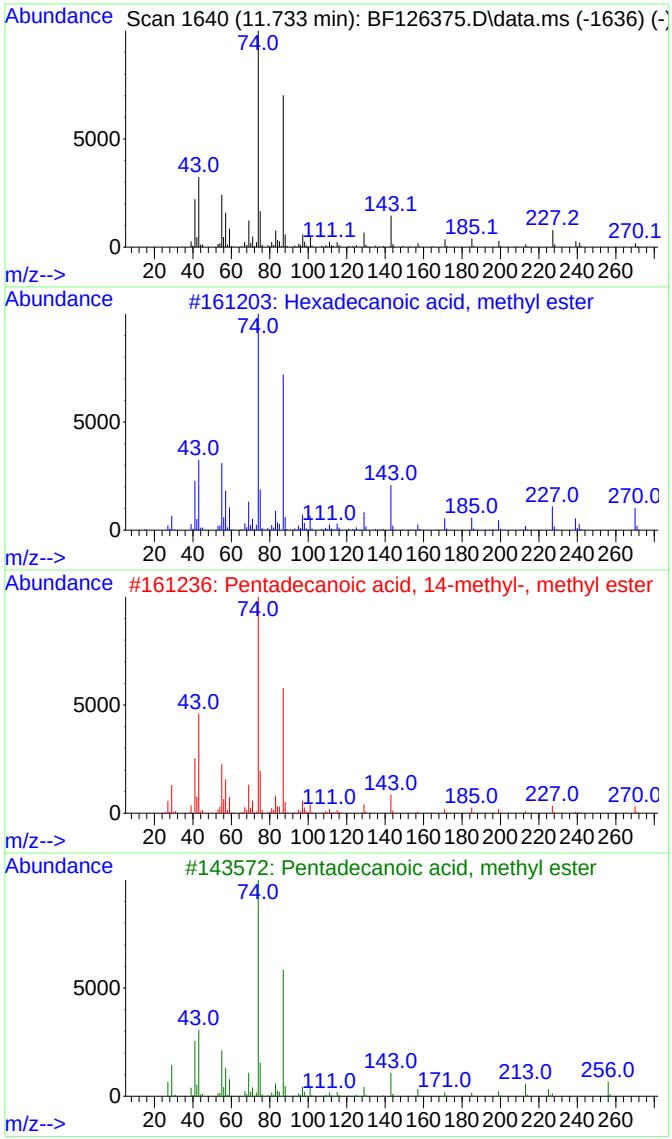
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF121521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

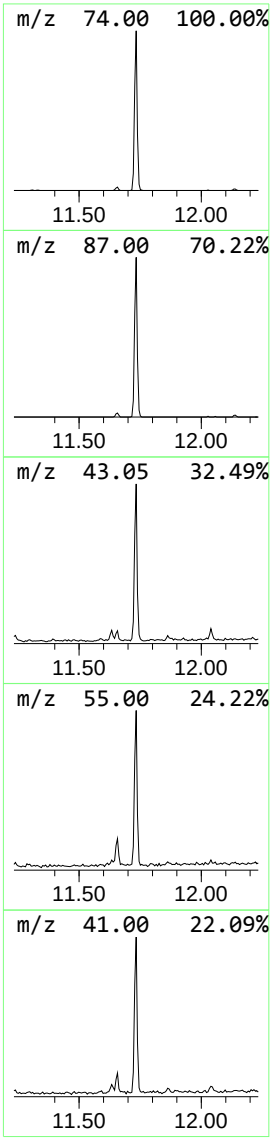
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Hexadecanoic acid, methyl e... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.733	18.78 ng	503837	Phenanthrene-d10	11.333

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	97
2	Pentadecanoic acid, 14-methyl-, ...	270	C17H34O2	005129-60-2	96
3	Pentadecanoic acid, methyl ester	256	C16H32O2	007132-64-1	90
4	Tridecanoic acid, methyl ester	228	C14H28O2	001731-88-0	87
5	Dodecanoic acid, methyl ester	214	C13H26O2	000111-82-0	86





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122721\
Data File : BF126375.D
Acq On : 28 Dec 2021 1:20
Operator : JU/CG
Sample : M5235-01 5X
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
HD-02-122321

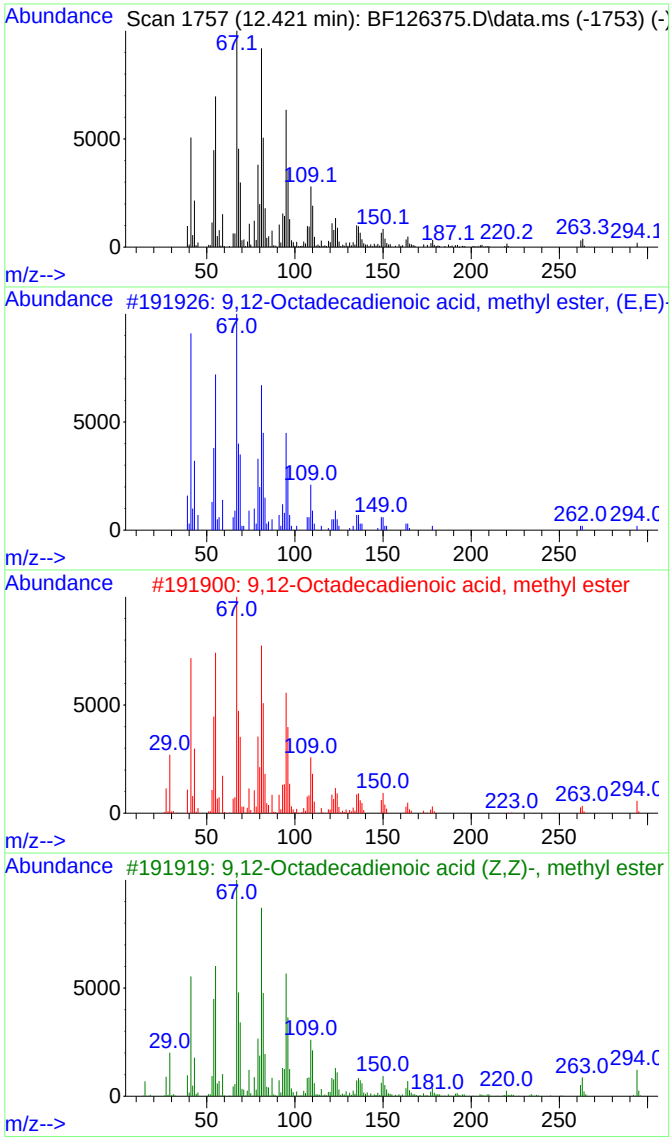
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF121521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

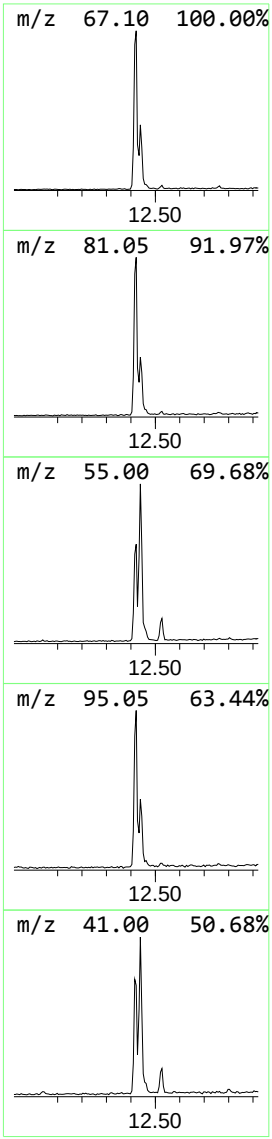
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 9,12-Octadecadienoic acid, ... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.421	33.16 ng	889608	Phenanthrene-d10	11.333

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9,12-Octadecadienoic acid, methy...	294	C19H34O2	002566-97-4	99
2	9,12-Octadecadienoic acid, methy...	294	C19H34O2	002462-85-3	99
3	9,12-Octadecadienoic acid (Z,Z)-...	294	C19H34O2	000112-63-0	99
4	9,11-Octadecadienoic acid, methy...	294	C19H34O2	013038-47-6	95
5	9,12-Octadecadienoic acid (Z,Z)-	280	C18H32O2	000060-33-3	95





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Instrument :
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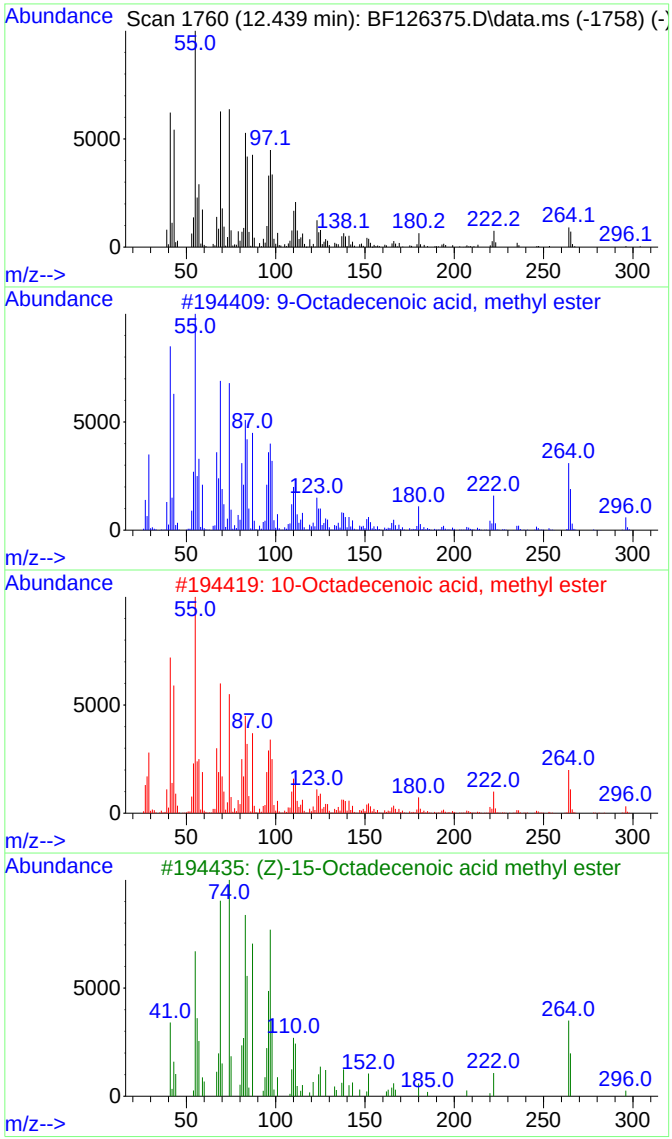
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF121521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

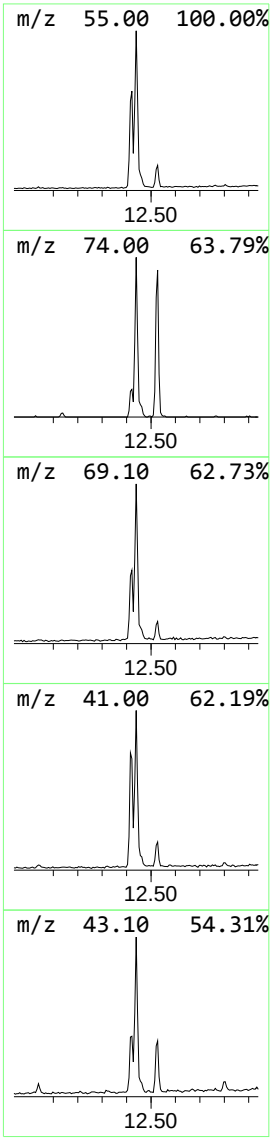
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 9-Octadecenoic acid, methyl... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.439	31.80 ng	853090	Phenanthrene-d10	11.333

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenoic acid, methyl ester	296	C19H36O2	002462-84-2	95
2	10-Octadecenoic acid, methyl ester	296	C19H36O2	013481-95-3	94
3	(Z)-15-Octadecenoic acid methyl ...	296	C19H36O2	1000427-69-3	93
4	9-Octadecenoic acid (Z)-, methyl...	296	C19H36O2	000112-62-9	91
5	11-Octadecenoic acid, methyl est...	296	C19H36O2	001937-63-9	91





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Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF121521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

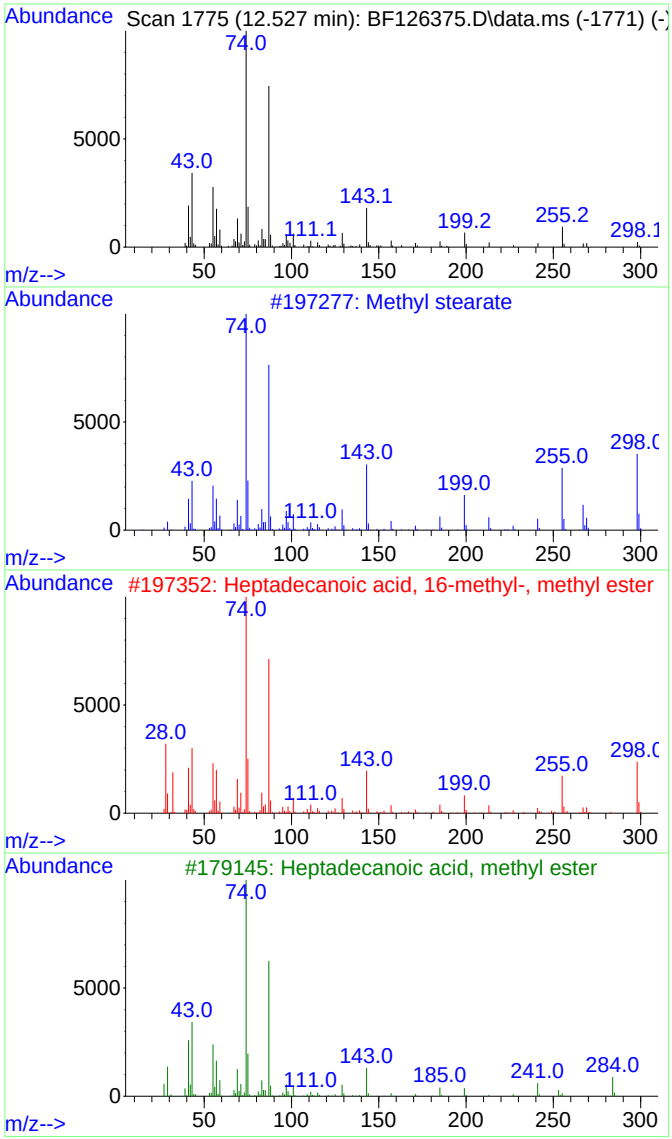
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

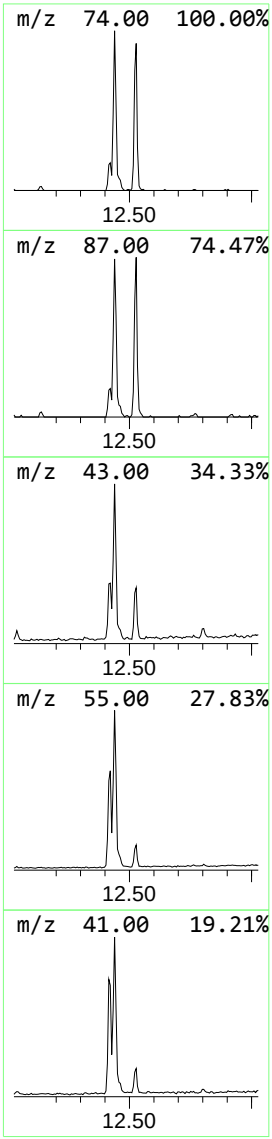
****

Peak Number 6 Methyl stearate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.527	8.83 ng	236899	Phenanthrene-d10	11.333

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Methyl stearate	298	C19H38O2	000112-61-8	96
2	Heptadecanoic acid, 16-methyl-, ...	298	C19H38O2	005129-61-3	90
3	Heptadecanoic acid, methyl ester	284	C18H36O2	001731-92-6	90
4	Pentadecanoic acid, 14-methyl-, ...	270	C17H34O2	005129-60-2	87
5	Methyl tetradecanoate	242	C15H30O2	000124-10-7	87





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Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
HD-02-122321

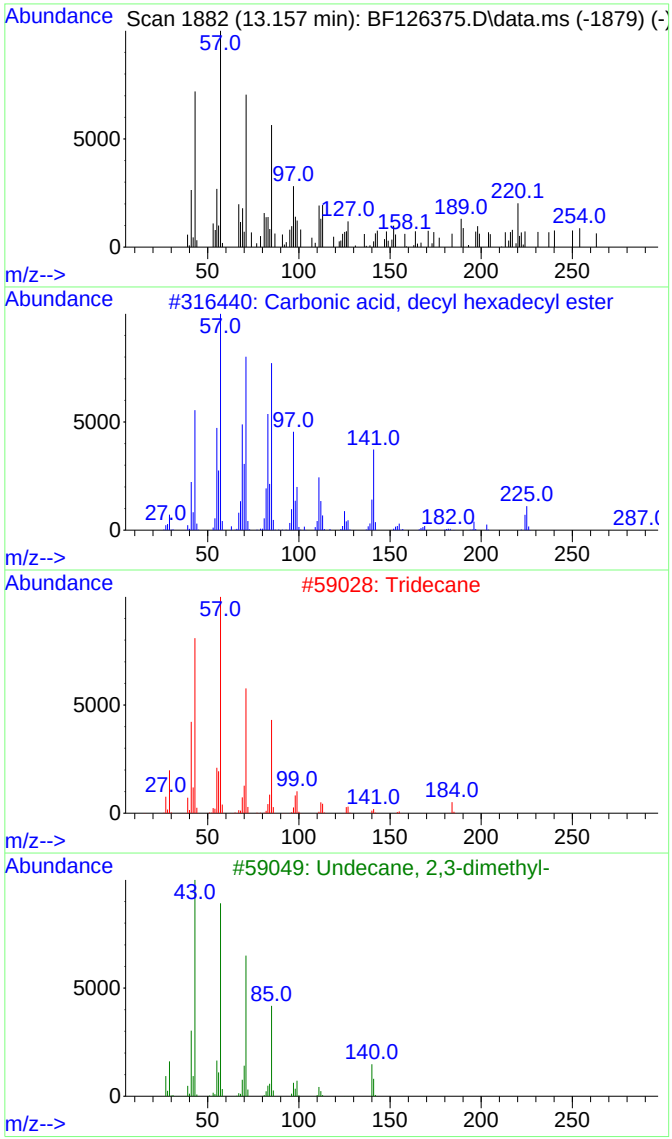
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF121521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

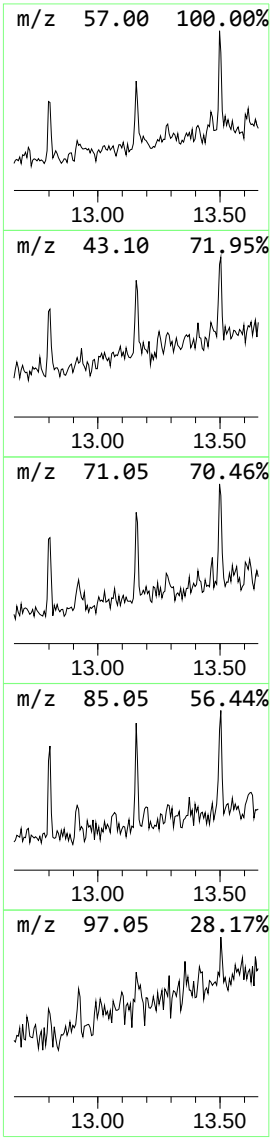
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Carbonic acid, decyl hexade... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.157	2.01 ng	60714	Chrysene-d12	13.974

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Carbonic acid, decyl hexadecyl e...	426	C27H54O3	1000383-16-5	50
2	Tridecane	184	C13H28	000629-50-5	38
3	Undecane, 2,3-dimethyl-	184	C13H28	017312-77-5	35
4	Tridecane, 1-iodo-	310	C13H27I	035599-77-0	35
5	5-Iodo-nonane	254	C9H19I	059456-19-8	35





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122721\
Data File : BF126375.D
Acq On : 28 Dec 2021 1:20
Operator : JU/CG
Sample : M5235-01 5X
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
HD-02-122321

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF121521.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
3-Penten-2-one,...	4.369	2.7	ng	67325	1	6.810	500818	20.0
2-Pentanone, 4-...	4.998	7.2	ng	181280	1	6.810	500818	20.0
Hexadecanoic ac...	11.733	18.8	ng	503837	4	11.333	536538	20.0
9,12-Octadecadi...	12.421	33.2	ng	889608	4	11.333	536538	20.0
9-Octadecenoic ...	12.439	31.8	ng	853090	4	11.333	536538	20.0
Methyl stearate	12.527	8.8	ng	236899	4	11.333	536538	20.0
Carbonic acid, ...	13.157	2.0	ng	60714	5	13.974	603526	20.0